Colloque du Programme National de l'INSU «Physique et Chimie du Milieu Interstellaire»

AstroRennes 2014

27-30 Octobre

Campus de Beaulieu
Université de Rennes 1

astrorennes2014.sciencesconf.org

Le milieu interstellaire (MIS) de la voie lactée à l'extragalactique

Des nuages moléculaires aux systèmes protoplanétaires

Origine de la complexité de la matière

Message du Conseil Scientifique de PCMI

Les études sur la physique et la chimie du milieu interstellaire connaissent un renouveau spectaculaire de par une conjonction d'évènements. D'un point de vue observationnel, les missions Herschel et Planck dans l'espace et les projets ALMA, NOEMA et NIKA au sol ouvrent de nouveaux horizons. Il est possible de faire de l'imagerie grand champ en radio-astronomie sub-millimétrique à plus ou moins grande résolution angulaire, de plus en plus souvent couplée à de la polarimétrie ou à l'observation simultanée de nombreuses raies.

Dans le même temps, la puissance des ordinateurs a permis

- à la simulation numérique de s'approcher significativement des conditions physiques et chimiques à l'œuvre dans le milieu interstellaire
- de traiter des systèmes de plus en plus complexes par calculs ab initio.

Par ailleurs, l'astrophysique de laboratoire française, propose de nombreuses expériences à la pointe pour produire et caractériser les analogues de la matière interstellaire et étudier les processus physiques fondamentaux régissant les interactions entre le gaz, les grains et leur environnement, dans un contexte où de grands instruments physiques (SOLEIL, GANIL, etc.) permettent de reproduire diverses conditions de rayonnement et où les données micro-physiques sont archivées dans des bases de données structurées.

Tout ceci permet de reconsidérer les questions au cœur de PCMI:

- Comment le milieu interstellaire évolue dans notre voie lactée et dans les galaxies plus ou moins lointaines ?
- Comment le gaz et la poussière se structurent, des nuages moléculaires aux systèmes protoplanétaires ?
- Quelle est l'origine de la complexité de la matière ?

Nous avons construit le programme du colloque pour permettre à notre communauté de débattre de ces questions et de réfléchir à la direction que nous souhaitons collectivement suivre dans les années à venir, dans un contexte où l'astrophysique de laboratoire cherche à se structurer au niveau au moins européen et où les financements récurrents font en partie place aux financements d'excellence très ciblés (ANR, ERC, ...).

Nous remercions la communauté pour s'être fortement investie dans ce colloque : il y a 150 inscrits pour environ 300 chercheurs émargeant à PCMI, il y a eu 72 propositions de communications orales pour 37 retenues. Nous remercions les invités d'avoir accepté de synthétiser des domaines souvent très larges et techniques en peu de temps. Nous remercions nos invités étrangers d'être venus de loin pour partager leurs expériences et savoir-faire. Nous remercions nos sponsors institutionnels (le CNRS, l'IRAM, l'Université de Rennes 1, l'Institut de Physique de Rennes, la métropole de Rennes et la région de Bretagne) ainsi que nos sponsors privés (Edwards, Pfeiffer-Vacuum, Continuum, MKS Instruments, Aerochop) sans qui ce colloque ne pourrait se tenir. Enfin, un grand merci au comité d'organisation local pour avoir réglé tous les détails pratiques de manière efficace.

Bon colloque à tous,

Jérôme, Karine, et Jean-Hugues pour le CS de PCMI.

Conseil Scientifique de PCMI

Jerome Pety, Institut de Radioastronomie Millimétrique (IRAM) Grenoble
Karine Demyk, Institut de Recherche en Astrophysique et Planétologie (IRAP), Toulouse
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Julie Nicolle, Institut de Physique de Rennes (IPR), Rennes
Emmanuelle Robin, Institut de Physique de Rennes (IPR), Rennes

Informations pratiques

Trajets transport en commun

De la gare : prendre le métro ligne A jusqu'à République, puis le bus ligne n°C4 ou ligne n°6 jusqu'au campus Beaulieu, arrêt Beaulieu/Tournebride

De l'arrêt de bus Beaulieu/Tournebride, marcher 2 minutes pour accéder au bâtiment 1
(cf plan du campus de Beaulieu)

Info pratique : En début et fin de journée, le bus n°41ex relie la gare et le campus Beaulieu en moins de 10 minutes.

Consulter les plans et les horaires des lignes sur le site de la STAR : http://www.star.fr/

Du campus au centre de Rennes / République : prendre le bus ligne n°4 ou ligne n°6

Plan de Rennes

Plan du campus

Physique et Chimie du Milieu Interstellaire

AstroRennes 2014

27-30 Octobre

Programme

lundi 27 octobre 2014

09h00-09h50 Accueil et inscription

09h50-10h00 A.Canosa Introduction Amphithéâtre A

Magnetic field in the ISM

10h00-10h25 K. Ferrière Magnetic field in the ISM: Observations (Planck, PILOT, LOFAR) and simulations
10h25-10h45 F. Levrier Polarized thermal dust emission from Planck
10h45-11h05 M. Alves The magnetic field structure in the Rosette nebula

Star formation

11h05-11h30 F.X. Désert (Sub-)mm wide-field observations at medium angular resolution: 30m + CCAT + APEX
11h30-11h50 A. Rivera The Role of Environment in the Formation and Evolution of ISM Filaments
11h50-12h10 P. André Probing the universality of interstellar filamentary structure: From Herschel to ArTéMiS and beyond

12h10-13h30 *Déjeuner - buffet sur place*

Observational constraints on dust modeling

13h30-13h50 D. Paradis Modeling and predicting the shape of the far-infrared/submillimeter emission in ultra-compact HII regions and cold clumps
13h50-14h10 L. Fanciullo Planck observations challenge existing dust models
14h10-14h30 C. Lefèvre Dust properties inside molecular clouds from coreshine modeling and observations
14h30-14h50 M. Koehler Self-consistent modelling of dust growth from the diffuse to dense ISM
14h50-15h20 Discussion 1: Scientific results from Herschel/Planck and analysis of open questions for the scientific community, chaired by **M. Gérin** (LERMA) and **I. Ristorcelli** (IRAP)

15h20-15h50 *Pause café*

Gas phase studies (1)

15h50-16h15 F. Lique State-to-state molecular collisions: progresses and prospects
16h15-16h35 Y. Scribano Quantum dynamics study of rate constant for a reactive collision of astrophysical interest : the $D^+ + H_2$ reaction
16h35-17h00 S. Le Picard Gas phase chemical kinetics: experimental advances and prospects
17h00-17h20 J.C. Loison The interstellar gas-phase chemistry of HCN and HNC
17h20-17h40 M. Fournier Measurement of rate constants for reactions of C_3N with small molecules using the CRESU technique
17h40-18h00 A. Bellili VUV spectroscopy and photophysics of interstellar and prebiotic molecules
18h00-18h20 X. Michaut Experimental investigations on nuclear spin-states equilibration of hydrogenated molecules at low temperature gas-solid interface

18h20-19h20 Visit of the CRESU experiments - Institut de Physique de Rennes - bât. 11C

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Gas phase studies (2)

09h00-09h20 K. Hickson CRESU studies of the reactivity of atomic nitrogen at low temperature

09h20-09h40 C. Sleiman Experimental and Theoretical Study between CN radical and Acetonitrile CH_3CN Relevant to Astrochemical Environments

09h40-10h00 L. Margulès Submillimeter-wave spectroscopy of nitrogen containing molecules of astrophysics interest

10h00-10h15 M.L. Dubernet The Virtual Atomic and Molecular Data Centre (VAMDC): Science Use Cases and the VAMDC Consortium

From protostars to protostellar disks and comets

10h15-10h35 B. Lefloch Exploring the Molecular Complexity of Protostellar Environments with ASAI

10h35-10h55 S. Maret Results of the CALYPSO survey of the youngest protostars: Chemistry, dynamics, and disk formation

10h55-11h25 *Pause café*

11h25-11h45 M. Gerin High resolution mapping of the B1b core : the interaction of two young protostars with their environment

11h45-12h10 V. Piétu (sub-)mm, high angular resolution observations of protoplanetary disks: PdBI/NOEMA & ALMA

12h10-12h35 D. Bockelée-Morvan Between ISM and protoplanetary disks: The molecular composition of comets (ROSETTA/PHILAE)

12h35-13h00 J. Tennyson Spectroscopy and chemistry of exoplanets

13h00-14h15 *Déjeuner - buffet sur place*

14h15-14h45 Discussion 2: Is there any limit for the molecular complexity in space? Multi-wavelength detection, and understanding the formation mechanisms, chaired by **Pierre Hily-Blant** (IPAG) and **L. Margulès** (PhLAM)

14h45-15h45 Sponsor presentations (Amphi A bât. 2)

15h45-17h15 *Pause café* + **Poster session 1**

Organisational aspects

17h15-17h40 E. Roueff The genesis of PCMI

17h40-17h50 J. Tennyson European Task Force for Laboratory Astrophysics (ETFLA)

17h50-18h00 F. Salama Laboratory Astrophysics Division of the American Astronomical Society (AAS/LAD)

18h00-19h00 Visit of the CRESU experiments - Institut de Physique de Rennes - bât. 11C

19h15-20h15 Conference grand public au Diapason :

«L'exploration de l'Univers, la révolution ALMA»

Maryvonne Gérin, Directrice du Laboratoire de Radioastronomie de l'École Normale Supérieure, Observatoire de Paris.

Physique et Chimie du Milieu Interstellaire

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Experiments on interstellar ices (1)

09h00-09h25 P. Theulé Chimie des glaces : formation des molécules complexes et photodésorption
09h25-09h45 P. Ghesquière Diffusion-limited reactivity in interstellar ice
09h45-10h05 J.B. Bossa UV laser desorption time-of-flight mass spectrometry of VUV photo-processed ices
10h05-10h25 M. Faure Hydrogen/deuterium exchanges in interstellar ice analogs
10h25-10h45 L. Krim Formation of hydroxylamine from ammonia and hydroxyl radicals. An astrochemically-relevant two-step mechanism

10h45-11h15 *Pause café*

Shock, PDRs, and HII regions

11h15-11h35 A. Gusdorf The environmental impact of irradiated shocks in the W28 A2 massive star forming region
11h35-12h00 A. Abergel The JWST project: Applications to PDRs or shocks
12h00-12h20 P. Pilleri High spatial resolution observations of key hydrocarbon species in the NGC 7023 PDR
12h20-12h40 O. Berné Dynamical properties of warm and dense photodissociation regions: from the interstellar medium to protoplanetary disks

12h40-13h50 *Déjeuner - buffet sur place*

13h50-14h10 P. Tremblin Impact of ionization compression on turbulent molecular clouds and dating of OB associations
14h10-14h30 P. Gratier Bright CO clumps resulting from the interaction of the HD34078 runaway star with the diffuse IC405 nebula
14h30-14h55 A. Decourchelle X-ray observations of supernova remnants and the future European X-ray observatory Athena
14h55-15h25 Discussion 3: Star formation yields, 3D structure of the ISM: The role of magnetic field, turbulence, stellar feedback and cosmic rays, chaired by **F. Boulanger** (IAS) and **B. Commercon** (CRAL)

15h25-16h20 *Pause café* + **Poster session 2**

H_2 formation and extragalactic ISM

16h20-16h45 J. LeBourlot Formation of H_2 in the Galaxy, sub-metallic galaxies, and the early Universe
16h45-17h05 E. Bron Dust temperature fluctuations and surface chemistry: H_2 formation
17h05-17h30 C. Bot What does the study of nearby galaxies teach us about the ISM processes?
17h30-17h50 A. Remy-Ruyer Probing the impact of metallicity on the dust properties in galaxies

18h30-19h30 Visit of Rennes center

19h30-23h00 Conference dinner at Lecoq Gadby

Physique et Chimie du Milieu Interstellaire

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jeudi 30 octobre 2014

Experiments on interstellar ices (2)

09h00-09h25 S. Morisset Formation of molecules at the gas-surface interface: experimental and theoretical advances

09h25-09h45 H. Chaabouni Water formation through O_2+D pathway on cold silicates and amorphous water surfaces of interstellar interest

Dust formation and lifecycle

09h45-10h10 M. Godard Hydrogenated Amorphous Carbons: evolution of interstellar carbon dust

10h10-10h35 F. Salama The formation of solid particles from their gas-phase molecular precursors in cosmic environments

10h35-10h55 M. Guélin Small scale structure of IRC+10216: a key to time dependent chemistry

10h55-11h25 *Pause café*

11h25-11h50 C. Joblin PAHs from circumstellar environments to the interstellar medium. The Nanocosmos project

11h50-12h20 Discussion 4: Nucleation, coagulation, clustering processes, photolysis, formation and desorption of ices. Impact on ISM and protoplanetary disks, chaired by **J.H. Fillion** (LERMA) and **K. Demyk** (IRAP)

12h20-13h30 *Déjeuner - buffet sur place*

ISM phases in and model of our Galaxy

13h30-13h55 V. Wakelam 3D interstellar chemo-physical Evolution (3DICE)

13h55-14h20 J. Black Visible and near-infrared spectroscopy of interstellar matter with ground-based instruments

14h20-14h40 F. LePetit The flux of cosmic rays and the physical conditions in the Central Molecular Zone of our Galaxy inferred by H_3^+

14h40-15h00 S. Vaupré Cosmic-ray induced ionization of a molecular cloud shocked by the W28 supernova remnant

15h00-15h20 P. Lesaffre Attempts at characterizing the structures of high dissipation in the interstellar medium

15h20-15h35 *Pause café*

15h35-16h00 L. Cambresy What do we learn from surveys (GAIA, PANSTARR, VISTA, etc) concerning the structure and phases of the ISM (3D ISM, extinction curve and diffuse bands studies)

16h00-16h25 F. Bournaud What is the status of the current models of our Galaxy?

16h25-16h40 Languignon SO5 - Plateforme MIS & Jets

16h40-17h10 Discussion 5: How to model the physics/chemistry of ISM (1D PDR, 1D shock, 3D MHD, 3D radiation transfer,...). Impact of the accuracy limitations and predictive capability of models? chaired by **F. Le Petit** (LERMA) and **P. Lesaffre** (LERMA).

Précisions programme

lundi 27 et mardi 28 octobre

Visite expérience CRESU - Institut de Physique de Rennes- Bâtiment 11C

Lundi de 18h20-19h20 et mardi de 18h00-19h00 */ sur inscription / (cf plan campus Beaulieu)*

mardi 28 octobre

19h15 : Conférence Grand Public au Diapason sur le Campus de Beaulieu

Entrée Libre

«L'exploration de l'Univers, la révolution ALMA»

Maryvonne Gérin, Directrice du Laboratoire de Radioastronomie de l'École Normale Supérieure, Observatoire de Paris.

Résumé : Depuis la détection du premier signal en ondes radio depuis l'espace, l'exploitation des signaux dans les gammes de fréquences centimétriques et millimétriques en astrophysique s'est largement répandue.
L'interféromètre ALMA, un ensemble de 66 antennes sur le plateau d'Atacama au Chili, est le dernier instrument mis en service. Il apporte des capacités inédites pour l'étude de l'univers, depuis les objets du système solaire jusqu'aux galaxies les plus lointaines.
Cet exposé présentera l'instrument, le cheminement scientifique qui a conduit à le réaliser et une sélection des premiers résultats. ALMA a déjà obtenu des résultats spectaculaires dans le domaine de la formation des étoiles et des planètes en offrant une vision détaillée des régions obscures où se forment ces objets, inaccessibles à l'observation directe avec des télescopes opérant dans les longueurs d'onde visibles.
L'analyse des mesures effectuées avec ALMA fait appel aux résultats les plus actuels en physique moléculaire et nécessite une collaboration étroite entre astrophysiciens, physiciens et chimistes.
Des exemples issus des travaux des équipes françaises seront présentés.

mercredi 29 octobre

18h30-19h30 : Visite guidée du vieux Rennes */ sur inscription*

Rendez-vous devant le beffroi de la mairie à 18h30

La visite se termine à 19h30 rue d'Antrain au niveau du restaurant Lecoq Gadby

19h30-23h : Diner de Gala au restaurant Lecoq Gadby

156 Rue d'Antrain - 35700 Rennes - 02.99.38.05.55

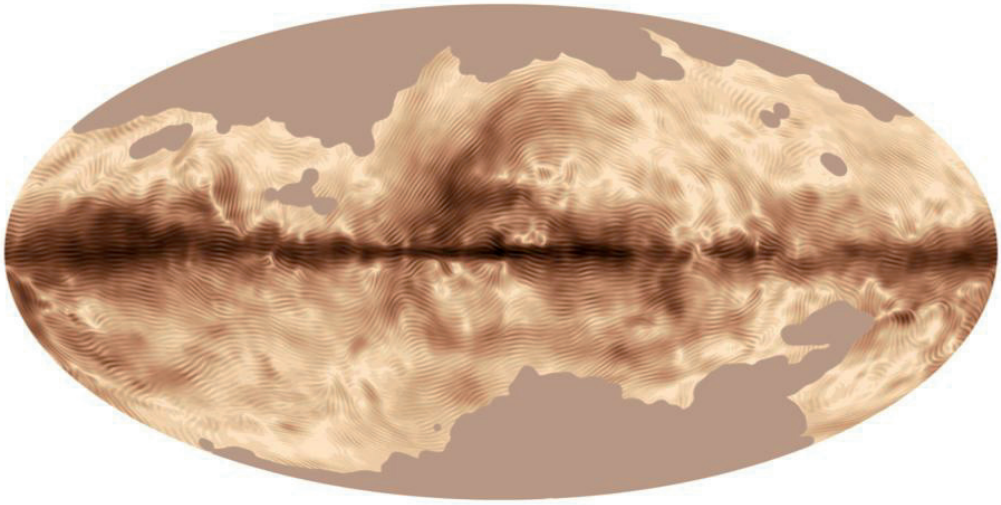
Contributions orales

Polarized thermal dust emission from *Planck*.

F. Levrier[1], on behalf of the *Planck* collaboration.

[1] *LERMA/LRA, ENS Paris et Observatoire de Paris, 24 rue Lhomond, 75231 Paris Cedex 05 – France*

The *Planck* satellite has mapped the polarized microwave and submillimetre sky (from 30 to 353 GHz) with unprecedented sensitivity and angular resolution. This wealth of data sheds new light on the polarization of Galactic foregrounds, especially that of thermal emission from aligned aspherical dust grains, which dominates the polarized cosmic microwave background (CMB) at the high end of the *Planck* frequency range. I will present the first results from the current analysis of *Planck* polarization data related to thermal dust emission. The *Planck* polarization data is scheduled to be made publically available in the fall of 2014.



Galactic polarization at 353 GHz (credits : ESA and the *Planck* collaboration)

Références

[1] Planck intermediate results. XIX. An overview of the polarized thermal emission from Galactic dust, arXiv:astro-ph 1405.0871

[2] Planck intermediate results. XX. Comparison of polarized thermal emission from Galactic dust with simulations of MHD turbulence, arXiv:astro-ph 1405.0872

[3] Planck intermediate results. XXI. Comparison of polarized thermal emission from Galactic dust at 353 GHz with optical interstellar polarization, arXiv:astro-ph 1405.0873

[4] Planck intermediate results. XXII. Frequency dependence of thermal emission from Galactic dust in intensity and polarization, arXiv:astro-ph 1405.0874

The magnetic field structure in the Rosette nebula

M.I.R. Alves[1], on behalf of the Planck Collaboration

[1] *IAS, Institut d'Astrophysique Spatiale, Université Paris XI, 91405, Orsay Cedex – France*

Planck has mapped the dust polarized emission over the whole sky, making it possible to trace the Galactic magnetic field structure that pervades the interstellar medium. We combine polarization data from *Planck* with rotation measure observations towards a massive star forming region, the Rosette nebula in the Monoceros molecular cloud, to study its magnetic field structure and the impact of an expanding HII region on the morphology of the field. *Planck* observations show a distinct magnetic field structure in the nebula compared to that of the surrounding medium, as a result of stellar feedback. The change in the magnetic field structure is accompanied by low values of the polarization fraction, below 5%, relative to the much higher intrinsic polarization of dust grains, 19%. We compare the radio and *Planck* observations with the prediction from a model of spherical expansion of an HII region in a uniform medium, to derive the three-dimensional structure and amplitude of the magnetic field.

Magnetic field in the ISM: Observations (Planck, PILOT, LOFAR) and simulations

Katia Ferrière[1]

[1] *IRAP, Université de Toulouse, CNRS, 9 avenue du Colonel Roche, BP 44346, F-31028 Toulouse Cedex 4, France*

I will review the main observational properties of interstellar magnetic fields in the disk and halo of our Galaxy. These properties are inferred from a variety of observational methods, including synchrotron emission, Faraday rotation, Zeeman splitting, and dust polarization. I will discuss each of these methods in some detail and explain what it has taught us about the strength, the direction, and the spatial structure of interstellar magnetic fields in our Galaxy, laying the emphasis on the most recent advances and on the expected contributions from upcoming instruments. I will also discuss the present status of numerical simulations and see how their predictions square with current observations.

The Role of Environment in the Formation and Evolution of ISM Filaments

Alana Rivera-Ingraham[1,2], Isabelle Ristorcelli[1,2], Mika Juvela[3] and the Galactic Cold Cores Collaboration.

[1] *Université de Toulouse; UPS-OMP; IRAP; Toulouse - France*

[2]*CNRS; IRAP; 9 Av. Colonel Roche, BP 44346, F-31028 Toulouse cedex 4 - France*

[3]*Department of Physics, P.O. Box 64, FI-00014, University of Helsinki – Finland*

The observed association of filaments with prestellar and protostellar objects has made these structures a priority target in the investigation of the earliest stages of core and star formation. Recent studies point towards a scenario in which these cores are formed by gravitational fragmentation of supercritical filaments (linear mass $M_{line} > 16.5\ M_o$/pc; e.g., [1]) with quasi-universal widths of ~0.1 pc [2][3]. In this work we have aimed to constrain the role of environment in filament formation and a possible evolution to supercritical filaments. The Herschel datasets of the Galactic Cold Cores Key Programme, covering a range of Galactic locations and distances, allows for a statistical study of filamentary properties in a range of environmental conditions.

Filaments were extracted from these fields with the *getfilaments* algorithm. Their column density structure was characterized based on the relative contributions from a 'core' component, represented by a Gaussian, and a 'wing' component, dominated by the power-law behaviour of the Plummer-like function. In the context of gravitationally-dominated evolution, we find that (sub)critical filaments could increase their total linear mass by increasing that of their core and wing components while decreasing their M_{line} (core) /M_{line} (wing) ratio. Both filament components appear to be linked to local environment, with filaments at higher background levels systematically reaching higher core and wing masses. The distribution of core and wing-dominated filaments suggests a wing origin probably linked to accretion, which is dependent on the mass of the core component and the availability of material.

Results are in good agreement with previous Herschel observations and theoretical models of filament formation ([4], [5], [6]), supporting an accretion-based evolutionary process. Supercritical filaments are formed from subcritical, contracting, self-gravitating filaments with a minimum core component close to criticality (M_{line} (core) $>6M_o$/ pc). Formation of such star-forming filaments would be aided by a dense environment with $A_V \gtrsim$ 3 mag. This emphasizes the need for triggering, or an alternative (dynamical) external event, in order to bypass the limitations of gravity in the most extreme conditions: star-formation in diffuse high-galactic latitude environments, and high-mass star formation.

[1] André, P., Men'shchikov, A., Bontemps, S., et al. 2010, A&A, 518, L102
[2] Arzoumanian, D., André, P., Peretto, N., & Könyves, V. 2013,A&A, 553, A119
[3] Arzoumanian, D., André, P., Didelon, P., et al. 2011, A&A, 529,L6
[4] Fischera, J., & Martin, P. G. 2012, A&A, 542, A77
[5] Heitsch, F. 2013, ApJ, 769, 115

Probing the universality of interstellar filamentary structure: From Herschel to ArTéMiS and beyond

Philippe André[1]

[1] *Laboratoire AIM, CEA Saclay, Orme des Merisiers – Bât. 709, 91191 Gif-sur-Yvette Cedex*

Herschel imaging surveys of Galactic molecular clouds have emphasized the quasi-universality of the filamentary structure of the cold ISM and the role of filaments in the star formation process (e.g. André et al. 2014 for a review). I will briefly summarize the Herschel results and will discuss on-going and future follow-up work on this topic. In particular, I will present initial results obtained with the new ArTéMiS submm camera on the APEX telescope at 350 microns (cf. André et al. 2008 and Hill et al. 2012 for very first results with the prototype camera P-ArTéMiS).

References

[1] André Ph., Di Francesco, J., Ward-Thompson, D., Inutsuka, S., Pudritz, R.E., Pineda, J., Review Chapter for Protostars and Planets VI, Eds. H. Beuther et al. , in press (2014) (astro-ph/1312.6232)
[2] André, Ph., Minier, V., Gallais, P. et al., A&A, 490, L27 (2008)
[3] Hill, T., André, Ph., Arzoumanian, D. et al., A&A, 548, L6 (2012)

(Sub-)mm wide-field observations at medium angular resolution: 30m + CCAT + APEX

F.-Xavier Désert[1]

[1] *IPAG: Institut de Planétologie et d'Astrophysique de Grenoble*
Univ. Grenoble Alpes, CNRS, IPAG, F-38000 Grenoble, France

Continuum observations in the millimetre domain have made much progress thanks to the advance of new detector technology. Cameras with ten thousand detectors are being built around the world so that the sky can be mapped with a speed increase by a factor 100 to 1000. New ground-based cameras bridge the gap between the whole sky (sub)millimetre survey by Planck and the far-infrared surveys by Herschel on one hand, and the high angular resolution observations (but with a small field-of-view) provided by interferometers such as Alma and Noema, on the other hand. The scientific cases for these cameras will be described, with a special emphasis on the new KID-based camera NIKA2 for the IRAM 30m telescope[1]. Other instruments which are in progress will be described too, such as Artemis, Laboca and Saboca on APEX, Bolocam on the LMT and the grandiose 25-m CCAT project. These cameras will make scientific advances in many areas including the solar system, surveys of galactic star forming regions, nearby galaxies, extragalactic deep surveys and the measurement of clusters of galaxies interacting with the Cosmic Microwave Background.

References

[1] nika2 web page: http://ipag.osug.fr/nika2

Dust properties inside molecular clouds from coreshine modeling and observations.

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Using observations to deduce dust properties, grain size distribution, and physical conditions in molecular clouds is a highly degenerate problem. The coreshine phenomenon, a scattering process at 3.6 and 4.5 μm that dominates absorption, has revealed its ability to explore the densest parts of clouds [1, 2]. We want to use this effect to constrain the dust parameters and investigate to what extent grain growth (at constant dust mass) inside molecular clouds is able to explain the coreshine observations (~100 sources). We aim to find dust models that can explain a sample of Spitzer coreshine data but we also look at the consistency with near-infrared data we obtained for a few clouds. We built a grid of dust models and investigated the key parameters to reproduce the general trend of surface brightnesses and colors of both coreshine and near-infrared observations with the help of a 3D Monte-Carlo radiative transfer code [3]. The grid investigates the effect of coagulation upon spherical grains up to 5 μm in size derived from the DustEm diffuse interstellar medium grains [4]. Fractal dimension, porosity, ices, and a handful of classical grain distributions were also tested. We used the near– and mostly mid–infrared colors as strong discriminants between dust models.

For starless cores, where detected, the observed 4.5 μm/3.6 μm coreshine intensity ratio is always lower than ~0.5 which is also what we find in the models. Embedded sources can lead to higher fluxes (up to four times greater than the strongest starless core fluxes) and higher coreshine ratios (from 0.5 to 1.1). This ratio enhancement is readily explained by the reddening of the sources, especially with Class 0 and 0/I objects, that changes the local balance of the radiation field at the mid–infrared wavelengths. Normal interstellar radiation field conditions are sufficient to find suitable grain models at all wavelengths for starless cores. The standard interstellar grains are not able to reproduce observations and, due to the multi-wavelength approach, only a few grain types meet the criteria set by the data. Porosity does not affect colors while fractal dimension helps to explain mid–infrared colors but does not seem to reproduce near–infrared observations without a mix of other grain types.

We will present the potential of combined near– and mid–infrared wavelengths to reveal the nature and size distribution of dust grains. Careful assessment of the environmental parameters (global interstellar and background fields, embedded or nearby reddened sources) is required to validate this new diagnostic and will be discussed.

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Modeling and predicting the shape of the far-infrared/submillimeter emission in ultra-compact HII regions and cold clumps

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Dust properties are likely affected by the environment in which dust evolve. For instance, some analyses of cold clumps (7 K- 17 K) lead to favor the aggregation process in dense environments [1]. However, the study of warm (30 K-40 K) dust emission at long wavelength (λ>300 μm) has been limited by the difficulty in combining far infared-millimeter (FIR-mm) spectral coverage and high angular resolution to observe warm dust grains.

Using Herschel data from 70 to 500 μm, as part of the Herschel infrared Galactic (Hi-GAL) survey associated to 1.1 mm data from the Bolocam Galactic Plane Survey (BGPS), we compare emission in two types of environments: ultra-compact HII (UCHII) regions and cold molecular clumps (denoted as cold clumps). This comparison allows us to test models of dust emission in the FIR-mm domain used to reproduce emission in the diffuse medium [2], in these environments, and to check their ability to predict the dust emission in our Galaxy.

We determine the emission spectra in twelve UCHII regions and twelve cold clumps, and derive the dust temperature (T) using the recent two-level system (TLS) model (Mény et al., 2007) with three sets of parameters, and the so-called T-β (Temperature-dust emissvity index) phenomenological models, with β set up to 1.5, 2 and 2.5.

The applicability of the TLS model in warm regions has been tested for the first time. This analysis points out distinct trends in the dust emission between cold and warm environments, visible through changes in the dust emissivity index. However, with the use of standard parameters, the TLS model is able to reproduce the spectral behavior observed in cold and warm regions, by the only change of the dust temperature, as opposed to a T-β model which requires the knowledge of β.

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Self-consistent modelling of dust growth from the diffuse to dense ISM

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Dust grains play a crucial role in many physical and chemical processes in the ISM. Their properties influence, for example, the formation and temperature of the major molecules in molecular clouds. It is therefore important to characterise the grain size, structure, shape and material composition in all phases of the ISM. Observations of the dust SED and extinction point towards variations in dust properties in the transition from the diffuse to denser ISM. The observed SEDs show a decrease in colour temperature, an increase in the spectral index and an increase in emissivity in the far-IR and sub-mm [1,2].

We explain these variations by accretion and coagulation processes. Our modelling is based on the diffuse-ISM dust model of [3] and [4], for which we allow for the accretion of carbonaceous and ice mantles as well as coagulation into aggregates. We use DDA [5] in order to derive the optical properties of these evolved grains and DustEM [6] in combination with the CRT radiative transfer code [7] to determine the SEDs which we compare to observations. The variations in the optical properties due to dust evolution are able to describe the observed changes in the SED from the diffuse to dense ISM with Av<10 [8].

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Planck observations challenge existing dust models

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The newly available *Planck* data provide a full sky view of the Milky Way in the submillimetre at a resolution of 5 arcmin. These new constraints on the spectral energy distribution (SED) of large (0.1 μm) dust grains were analyzed using models (Draine+Li 2007, Compiègne+2011 and Jones+2013) which include a distribution of carbonaceous and silicate grains, tailored to reproduce pre-*Planck* observational constraints.

We show that fitting the *mean* dust SED with the Draine & Li model overpredicts the Av, and therefore the dust mass, by a factor ~2, while the Compiègne model, and especially the Jones model, are closer to the data (within 50% and 20%, respectively).

By normalizing the SED to the extinction measured toward 200,000 quasars from SDSS, we provide a family of 8 diffuse ISM SEDs of the dust thermal emission which differ in their temperature and emissivity per unit magnitude extinction. This confirms that the dust emission properties vary in the diffuse ISM, even at the very low column densities probed here (Av < 0.5). By comparing dust in emission (SED) with dust in extinction (Av), this study is exempt of caveats that arise when normalizing the SED by the gas column density as estimated from H I and CO emission.

While the mean SED is reasonably fitted by the Jones model, none of the models (which all assume fixed dust optical properties) can reproduce the variations observed in this family of SEDs.

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Discussion 1:

Scientific results from Herschel/Planck and analysis of open questions for the scientific community

chaired by

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The interstellar gas-phase chemistry of HCN and HNC

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We review the chemistry involving HCN and HNC in dark molecular clouds to elucidate new chemical sources and sinks of these isomers. We find that the most important reactions for the HCN-HNC system are Dissociative Recombination (DR) reactions of $HCNH^+$ ($HCNH^+ + e^-$), the ionic $CN + H_3^+$, $HCN + C^+$ reactions, HCN and HNC reactions with $H^+/He^+/H_3^+/H_3O^+/HCO^+$, the $N + CH_2$ reaction and two new reactions: H + CCN and C + HNC. We test the effect of the new rate constants and branching ratios on the predictions of gas-grain chemical models for dark cloud conditions. The rapid C + HNC reaction keeps the HCN/HNC ratio significantly above one as long as the carbon atom abundance remains high. However, the reaction of HCN with H_3^+ followed by DR of $HCNH^+$ acts to isomerize HCN into HNC when carbon atoms and CO are depleted leading to a HCN/HNC ratio close to or slightly greater than 1. This agrees well with observations in TMC-1 and L134N taking into consideration the overestimation of HNC abundances through the use of the same rotational excitation rate constants for HNC as for HCN in many radiative transfer models.

CRESU studies of the reactivity of atomic nitrogen at low temperature.

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At the present time, the reactivity of ground state atomic nitrogen ($N(^4S)$) at low temperature is poorly understood despite its importance for the chemistry of the interstellar medium and planetary atmospheres. This contribution will describe our recent experimental results on the kinetics of the reactions of atomic nitrogen with other small radical species such as OH, CN, CH, C_2 and C_2N to temperatures as low as 50 K. The experimental results will be compared with the results of quantum mechanical calculations and the future prospects for extending this method to investigate the reactions of other atomic radicals ($O(^3P)$, $H(^2S)$) will be discussed.

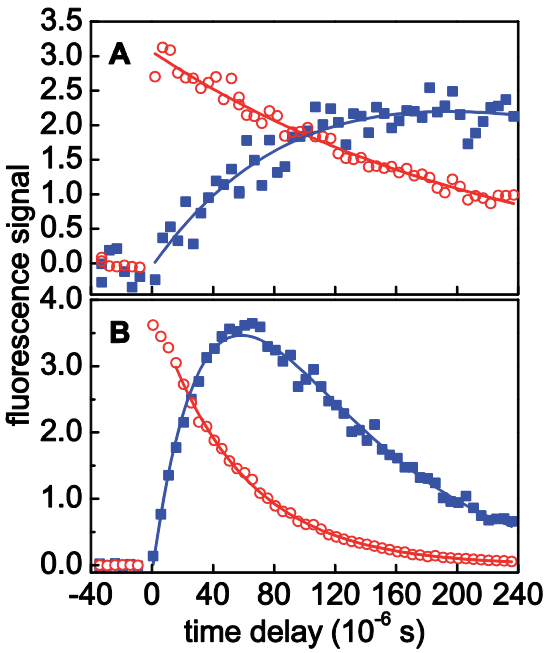

Fig. 1: (A) Exemplary temporal profiles at 147 K obtained for the N + OH → H + NO reaction with estimated [N] = 1.1 × 10^{14} atom cm^{-3}. ■NO($^2\Pi_{1/2}$) LIF signal. OOH($^2\Pi_{3/2}$) LIF signal. (B) As in (A) but with estimated [N] = 4.1 × 10^{14} atom cm^{-3}.

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The Virtual Atomic and Molecular Data Centre (VAMDC): Science Use Cases and the VAMDC Consortium

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The Virtual Atomic and Molecular Data Centre (VAMDC, http://www.vamdc.eu) has created an interoperable e-science infrastructure that currently inter-connects about 27 atomic and molecular databases with the number of connected databases increasing every year. The data can be queried and retrieved in a single format from a general portal (http://portal.vamdc.eu) and VAMDC is currently developing standalone tools to retrieve and handle the data. Currently VAMDC aims at improving the services for specific communities with up till now a strong emphasis on the physics and chemistry of the interstellar medium. The latest tools will be presented within the context of science use cases, in particular the SPECTCOL tool [1, 2] and the connection between VAMDC and the Virtual Observatory tools. In addition a general outline of the VAMDC Consortium activities will be provided. The paper aims at encouraging feedbacks from users and at showing the potential of the VAMDC Consortium for research, education, industry and outreach.

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Experimental and Theoretical Study between CN radical and Acetonitrile CH_3CN Relevant to Astrochemical Environments

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Acetonitrile (CH_3CN) has been detected in molecular clouds (Sgr B2) and in hot cores in regions of massive star formation. The CH_3CN abundance in these objects which was found to be 10^{-9} or larger was explained by evaporation of molecular material from ice mantles of interstellar grains.

The gas phase reactivity of CH_3CN was studied in the literature in the presence of OH, NO_3, Cl and CN. However, no data are available at temperatures below 256 K. For this reason, a kinetic study of acetonitrile in the presence of the CN radical in interstellar conditions has been carried out below 168 K using the CRESU technique (Cinétique de Réaction en Ecoulement Supersonique Uniforme / Reaction Kinetics in a Uniform Supersonic Expansion) which generates a low temperature flow reactor. The study was completed by a series of measurements in the temperature range 258 - 354 K using a cryogenic cell or the CRESU apparatus in its subsonic configuration. In order to determine the rate coefficient, Pulsed Laser photolysis (PLP) and Laser Induced Fluorescence (LIF) techniques have been used. A first laser produced CN radicals by photolysis of ICN at 266 nm, while the second one, delayed with respect to the photolysis pulse, probed the fluorescence of these radicals by excitation at 387 nm. The rate coefficients of the studied reactions were determined from the temporal evolution of the fluorescence signal as a function of the CH_3CN concentration.

Whereas at temperatures higher than 200 K, the rate coefficient presents a usual Arrhenius behavior, a dramatic increase by *two orders of magnitude* in the temperature range 168 – 123 K occurs. At temperatures lower than 120 K, the rate coefficient still increases but at a lower level, reaching a value of $(5.08\pm0.86)\times10^{-11}$ $cm^3molec.^{-1}s^{-1}$ at 23 K. Interestingly, the rate coefficient was no pressure dependent at room temperature whereas this was observed below 168 K indicating a very different reactive mechanism according to the temperature range. More specifically, at 132 K and 52 K, measurements indicated that the stabilization of the adduct was competing with tunneling through an activation barrier confirmed by theoretical calculations. At 132 K, the tunneling contribution was precisely determined to be $(2.04\pm0.12)\times10^{-12}$ $cm^3molec.^{-1}s^{-1}$ and seems to increase at lower temperatures. This is the first time that this kind of behavior is identified at very low temperature for the CN radical reactivity in the gas phase.

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Experimental investigations on nuclear spin-states equilibration of hydrogenated molecules at low temperature gas-solid interface

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We performed, within the GASOSPIN ANR project, experimental approaches and related calculations with the aim to investigate the dynamics of the nuclear spin states re-equilibration of hydrogenated molecules at very low temperatures. The motivation of this work is to understand the physical parameters that can play a role in the anomalies that are observed in the *Ortho-to-Para Ratios* (OPR) measured in comets and ISM. Different physical conditions ranging from very diluted matter to condensed phases were considered and discussed: molecules in the gas phase (H_2CO), molecules trapped in cryogenics matrices (H_2O, CH_4) or adsorbed on cold surfaces (H_2), molecules desorbing from cold surfaces (H_2) and finally solid-gas equilibrium at very low temperatures (CH_4, H_2O). In these different environments, we are now able to propose the dominant mechanism responsible for the nuclear spin conversion and estimate the characteristic time of conversion.

In this communication, we will focus on the recent progress we made concerning solid-gas interface and the observations we made in laboratory concerning OPR equilibration during deposition, residence and desorption from cold surfaces. Comparisons of the insight we can get from experiments dedicated to molecules like CH_4, H_2O and H_2 will be considered. Finally, perspectives about the influence of photodesorption will be given.

VUV spectroscopy and photophysics of interstellar and prebiotic molecules

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For many years, our group has been investigating the VUV spectroscopy and photophysics of large molecules of astrophysical and prebiotic interest. We have studied simple compounds like acetic acid, acetonitrile, acetamide, as well as molecules of more immediate biological importance such as nucleic acid bases [1]. Polyynes and cyano-polyynes have been investigated too since these linear carbon and nitrogen chain molecules are very important in the ISM and might act in prebiotic chemistry (see for example our recent work [2a,b]). An aerosol source for reactive and thermo-labile compounds has been developed since many bigger molecules of astrophysical or prebiotic importance are not easily vaporized [3]. We consider gas phase measurements as particularly necessary since they permit to measure the intrinsic photophysical properties of relevant molecules. Furthermore, comparison to quantum chemical calculations, where in most cases isolated molecules are studied, is straightforward. Complex molecules give us insight into the functioning of astrophysical objects because of their spectra which are highly instructive and the chemical network they constitute. Basic UV photophysical data are needed in order do understand and model the chemical evolution of such molecules.

We present here results from our last year's measurement campaigns at Soleil and Bessy where we studied especially aminoacetonitrile (H_2NCH_2CN) and acetyl cyanide (H_3CCOCN). H_2NCH_2CN, which is a direct precursor of glycine, has been detected in Sgr B2(N) in 2008. This detection has not been confirmed since, but this compound can be formed by Strecker-type reactions, pathways which are thought to be a solid scenario for the formation of amino acids in space. H_3CCOCN has not been detected yet in astrophysical objects. The formation of H_3CCOCN needs only bimolecular interaction of acetaldehyde and HCN (for example on grains). We also note that the lower homologue of acetyl cyanide, which is formyl cyanide (HCOCN) has been also detected in Sgr B2(N) in 2008.

At Soleil, we have measured photoelectron photoion coincidence (PEPICO) spectra from the IE up to 13.6 eV, which is the interstellar HI limit, using the newly developed DELICIOUS III

spectrometer available at the DESIRS beamline. This spectrometer allows for species selective spectroscopy which is of particular importance when studying unstable compounds. In Figure 1, we show the PEPICO photoionization efficiency spectrum (PEPICO-PIE) of H_3CCOCN where electrons with kinetic energies up to 3.36 eV are considered for the coincidence measurement.

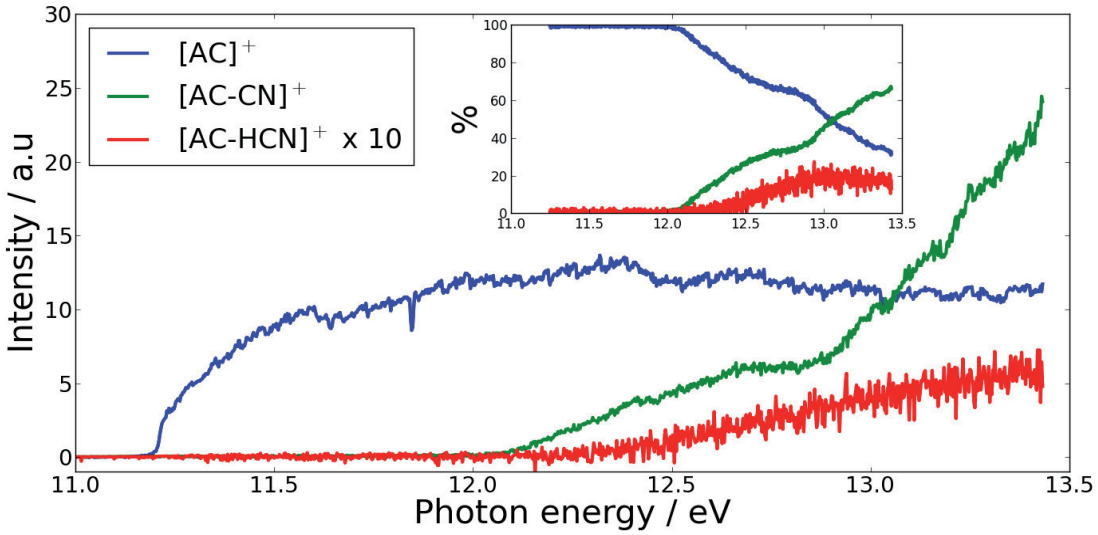

Figure1. PEPICO-PIE spectrum of acetyl cyanide H_3CCOCN (denoted AC). The intensity is normalized with respect to the incoming photon flux. The insert shows branching ratios of the three ions that can be formed (H_3CCOCN^+, H_3CCO^+, H_2CCO^+) as a function of photo excitation energy.

In Figure 1, besides the parent ion yield curve, two dissociative ionization pathways are observed corresponding to loss of CN and HCN of the parent molecular cation. In order to interpret our experimental data obtained using synchrotron radiation, we explored the ground potential energy surface (PES) of acetyl cyanide and of its cation using standard and recent explicitly correlated methodologies [see for example ref. 4]. These calculations include the enol tautomers which can be formed at excitation energies covered in our study. This allowed us to deduce accurate thermochemical data. We will present these calculations and deduce that unimolecular decomposition of H_3CCOCN^+ turns out to be very complex.

In this contribution, we will also present PEPICO-PIE spectra of aminoacetonitrile H_2NCH_2CN obtained using the same method. We will further present preliminary results from a campaign lead in June 2014 at Bessy II synchrotron radiation facility. There, the absolute VUV absorption spectra of H_3CCOCN, H_2NCH_2CN, and also propynal (HCCCHO) and isoacetonitrile (CH_3NC) have been studied for the first time at the U125/2 10m NIM beamline.

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Quantum dynamics study of rate constant for a reactive collision of astrophysical interest : the $D^+ + H_2$ reaction

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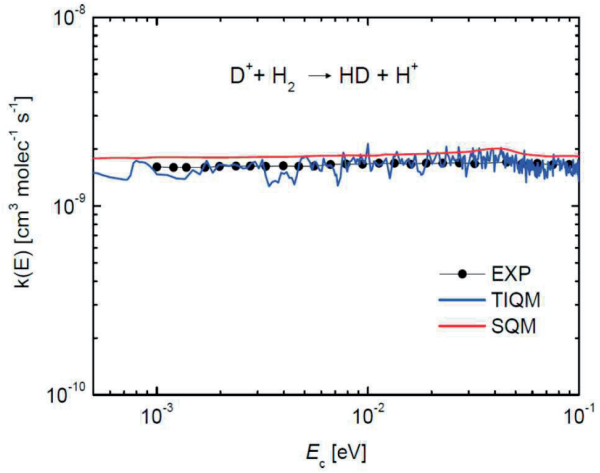
For chemistry networks describing the reactions for the early universe [1] and especially for accurate models of the enrichment of deuterated molecules observed, we need to know in detail many state-to-state rate coefficients. For instance, Glover and Abel [2] modeled the chemistry of H_2 and HD primordial gas using a chemical network consisting of 115 reactions between 16 species. Today most of the rate coefficients of interesting reactions are still unknown or with a poor accuracy. For example, the uncertainty about the rate coefficient for the reaction directly affects model predictions for the HD abundance and thereby the cooling rate of the primordial gas. It is therefore of astrophysical importance to determine an accurate value of these rates, and helping to understand the cooling requires a complete set of the state-to-state rate coefficients as well as the total rate coefficient. In this talk, I will illustrate how first principles calculations can furnish us the way to determine accurately the rate constants for low temperature (T<100 K). I will present the Time Independent Quantum Mechanical (TIQM) and Statistical Quantum Mechanical (SQM) results for the $D^+ + H_2$ reaction at low temperature using the accurate ab into potential energy surface of Velilla *et al*. determined for H^+_3 [3]. The state to state cross sections at low collisional energies and rate coefficients at low temperature have been computed [4,5,6,7] and compared to the available experimental data [8].



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Measurement of rate constants for reactions of C_3N with small molecules using the CRESU technique

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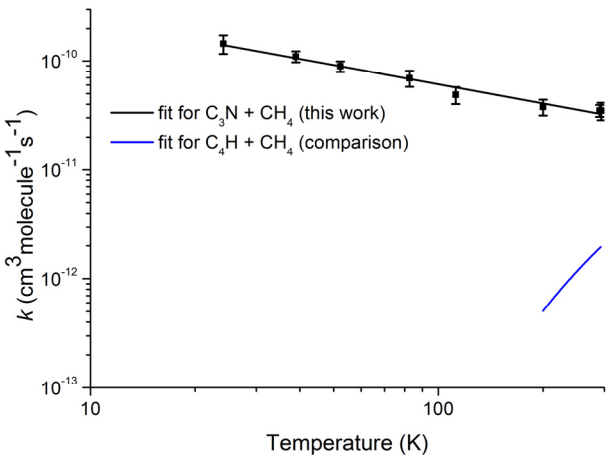
Since the first detection of radical species in the interstellar medium, attention has grown on polyynes, cyanopolyynes and corresponding radicals. This family encompasses a large number of species, from the very basic HCN to the largest linear compound to date, $HC_{11}N$. The key to the growth of larger members is the reactivity of intermediate sized ones, such as C_3N detected in multiple environments[1]. Astrochemical models were established for molecular clouds, planet atmospheres and circumstellar envelopes to explain the formation of these species.



Encouraged by previous work on C_4H[2] rate constant measurements over a large range of temperature and by using the CRESU (Cinétique de Réaction en Ecoulement Supersonique Uniforme) method we have measured the rate constants over the [24-300] K range for reactions of C_3N with C_nH_x compounds (n=1…3), CO, H_2, O_2 and NH_3. These results are the very first experimental data on C_3N reaction rates. Unlike expected from theoretical models and analogy with the isoelectronic species C_4H, the C3N proved extremely reactive at low temperature for almost all of these species, and quite reactive even at low temperature with H_2. The resulting measurements should be of significant interest for astrochemical models that essentially rely on similarity between compounds and extrapolation to fill the gap of insufficient experiment data.

Experimental data was acquired using pulsed laser photolysis on a synthesized precursor, BrC_3N, generating the radical in-flow and laser-induced fluorescence detection. LIF detection was based on experimental data acquired by Hoshina and Endo[3].

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Submillimeter-wave spectroscopy of nitrogen containing molecules of astrophysics interest

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Almost 30 nitrile molecules, which contain the cyano group (C≡N), have been detected in the interstellar medium (ISM) so far. The simplest of these nitriles, the cyano radical C≡N, was found in 1940 [1,2]. The most complex of all nitriles, $HC_{11}N$, having a total of 13 atoms, was detected in 1997 [3]. The vast majority of these nitriles have been detected in the dense molecular clouds Sgr A and B, and TMC-1 by means of their rotational spectra. The formation mechanisms of many of these compounds are not well understood.

In particular, many isocyanide compounds with a high kinetic instability, are poorly studied in laboratory. We investigated recently two of these compounds: diisocyanomethane, $CH_2(NC)_2$ [4], and allyl isocyanide, CH_2CHCH_2NC [5]. Following these studies we will report recent results about two others isocyanidse : ethylisocyanide, CH_3CH_2NC, and iso-cyanomethane, $NCCH_2NC$. Like many others complex organic molecules of astrophysical interest some of the nitriles exhibit large amplitude motions that make delicate the analysis of their spectra. This is the case of hydroxyacetonitrile, $HOCH_2CN$, and acetyl isocyanate, CH_3CONCO, which are currently studied. The latest results on these two molecules will be also presented.

This work was supported by the CNES and the Action sur Projets de l'INSU, PCMI. Part of this work was done within ANR-13-BS05-0008-02 IMOLABS

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State-to-state molecular collisions: progresses and prospects

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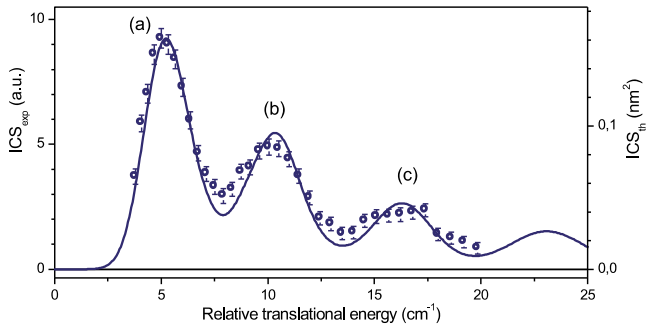
The Herschel satellite, the ALMA interferometer and the NOEMA telescope open new windows of observation for wavelengths ranging from far infrared to sub-millimeter with spatial and spectral resolutions previously unmatched. To make the most of these observations, an accurate knowledge of the collisional excitation rate coefficients of the interstellar molecules by the most abundant species (H, He, H_2) is needed. Indeed, accurate determination of molecular abundances relies on accurate collisional data. We present here the most recent advances in this area made by the French community.

First, we present the latest results for collisions between radicals (O_2, CN, C_2H), ions (HCO^+, N_2H^+) and H_2 [1-3]. For these systems, we will also expose detailed comparison between theoretical and experimental results showing the very good accuracy of the new data. Then, we will show the latest results obtained by the Hydrides ANR project on collisional excitation and chemistry of interstellar hydrides (OH, OH^+, CH, CH^+, NH, HCl) [4-5]. After this, we will also discuss the theoretical advances that have been made recently to take into account the excitation of bending modes of interstellar molecules (HCN, C_3) [6] but also to obtain reliable data for the collisional excitation of complex molecules (COM) [7].

Finally, we will show that the use of these new rate coefficients compared to the use of previous published ones significantly changes molecular abundances in molecular clouds.



$O_2(N_j=1_0)$+p-H_2 → $O_2(N_j=1_1)$+p-H_2 cross section: Experiments (open circles); theory (solid line)

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Gas phase chemical kinetics: experimental advances and prospects

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A major aim of astrochemistry is to determine the nature and abundance of molecules observed or suspected to be present in the interstellar medium. This necessitates the spectroscopic identification of the species as well as the construction of chemical models including large networks of elementary chemical and some physical processes. Experimental and theoretical efforts are needed to obtain the information about these processes which is required as input to the models. Of primary importance are the coefficients which describe the rate of all the elementary processes in the model, as well as the products of these processes.

In this contribution I will present recent advances and perspectives in the field of experimental kinetics that allow to determine: (i) the rate of various collisional processes of astrophysical interest over a wide range of temperatures, (ii) the nature of the products resulting from these collisions with, in some cases, complementary information such as their internal energy distribution or branching ratios of the major exit channels.

High resolution mapping of the B1b core : the interaction of two young protostars with their environment

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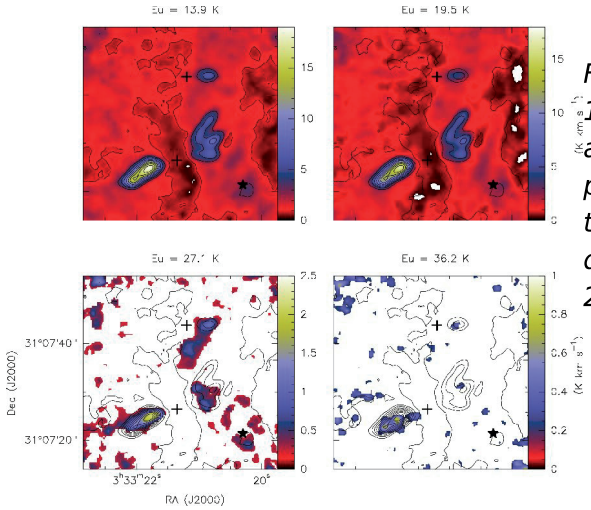
We present IRAM Plateau de Bure and 30m mapping observations of the Barnard 1b dense molecular core, combining detections of spectral lines of H_2CO and CH_3OH, as well as dust continuum emission at 2.2'' resolution (corresponding to ~500~AU). The two compact cores B1bN and B1bS are detected in the continuum at 2mm and 3mm, enabling an accurate analysis of their spectral energy distribution. We also detect molecular outflows associated with both cores. The outflow associated with B1bS presents bullets at velocities up to ~12 km/s from the core velocity, likely indicating variations in the accretion rate. The B1bN outflow is slower and more compact, with a dynamical age of less than 1000 years. A local peak of CH_3OH emission is detected near the position of the embedded protostar detected by Spitzer, possibly tracing the thermal evaporation of ice mantles. The 30m maps reveal the complex environment of the B1b core at large scale, with NH_2D tracing the cold cores and carbon chains a PDR on its east side.



Four methanol lines detected towards B1b at 145 GHz, with upper energy levels indicated above each map. The crosses show the positions of the B1bN and B1bS sources, and the star the position of the embedded source detected by Spitzer (S295, Jorgensen et al. 2006, ApJ 645, 1246).

Results of the CALYPSO survey of young solar-prototars: chemistry, dynamics and disk formation

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Class 0 protostars represent the earliest stage of the formation of a Sun-like star. This phase is crucial, as it determines the final mass of the star and the initial composition of the protoplanetary disk, that may eventually form planets. Yet, the chemistry and dynamics of these objects on a few hundred AUs scales - where disks are expected to form - is still poorly known, due to a paucity of millimeter observations at sub-arcsecond resolution. In fact, we still don't know how the progenitors of protoplanetary disks are formed during the youngest phases of protostellar formation. In this contribution, we present the results of a high-angular-resolution survey of 17 Class 0 protostars, obtained with the IRAM Plateau de Bure interferometer and the 30m telescope, as part of the CALYPSO Large Program (Continuum and Line Observations in Young Proto-stellar Objects; P.I. Philippe André). We discuss in detail three representative sources of our survey, NGC1333-IRAS2, NGC1333-IRAS4B and L1527. We find that IRAS2A and IRAS4B are associated with compact, yet resolved, emission from complex organic molecules (COMs). The size and the morphology of the emission suggest that they originate in a hot inner region heated by the protostar, in which the icy grain mantles evaporate (the so called hot corino). We also find an anticorrelation between the CO and N_2H^+ emissions in IRAS4B, which is likely caused by the destruction of N_2H^+ in the region of the protostar where CO ices evaporate. Our line observations also allow us to constrain the velocity field inside the protostellar envelopes. In IRAS4B, we detect an inverse P-Cygni line profile that indicates infall motions. In IRAS2, we detect some rotation on small scales, but no disk. Finally, in L1527 - where a protoplanetary disk has been recently detected - we detect rotation in several transitions, and we discuss the nature of the velocity profile as a function of the radius. A preliminary comparison of the properties of our Class 0 sample (chemical composition, presence of a disk) is also presented.

Exploring the Molecular Complexity in Protostellar Environments with ASAI.

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The Large Program ASAI carried out at the IRAM 30m telescope joins the efforts of several groups in Astrochemistry, in Spain and France, to address the question of our "chemical origins". Its goal is to obtain a complete census of the gas chemical composition, including pre-biotic molecules, and its evolution along the main stages of the star formation process, from prestellar cores and protostars to protoplanetary disks. This is achieved through highly sensitive and systematic spectral line surveys of a sample of sources illustrative of the various stages of protostellar evolution. The resulting data set is aimed to serve as a reference database for the astrochemical community: astronomers, chemists, and theoreticians.

We will present the first results obtained from the on-going data analysis. Some molecular lines remain to be identified, which will require a close collaboration with molecular spectroscopists. New molecular species have been discovered, both in prestellar cores and in protostellar shocks, opening the door to pre-biotic chemistry in these environments.

Spectroscopy and chemistry of exoplanets

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Exoplanets are now know to be ubiquitous, so naturally scientific enquiry is turning is turning towards characterisation. The obvious question to ask is what are exoplanets made of? Observational biases mean that it much easier to study spectroscopically (transiting) exoplanets close to their host star so these planets are hot.

At elevated temperatures the spectra of polyatomic molecules become extremely complicated with millions, or even billions, of transitions potentially playing an important role. The atmospheres of cool stars and "hot Jupiter" extrasolar planets are rich with molecules in the temperature range 1000 to 3000 K and their properties are strongly influenced by the infrared and visible spectra of these molecules. So far there are extensive, reliable lists of spectral lines for a number species including some stable diatomics, water, ammonia. Data is almost completely lacking for many key species.

The ExoMol project (www.exomol.com) aims to construct line lists of molecular transitions suitable for spectroscopic and atmospheric modelling of cool stars and exoplanets [1]. As huge numbers of lines are required. Line lists are therefore computed on the basis of a thorough quantum mechanical treatment of problem, which is tested against available laboratory data, rather than constructed experimentally. The methodology used to perform these calculations will be outlined.

Illustrative examples will be discussed including recent work on methane [2], for which we computed 10 billion lines, and water.

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(sub-)mm, high angular resolution observations of protoplanetary disks: PdBI/NOEMA & ALMA

Vincent Pietu

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Between ISM and protoplanetary disks: The molecular composition of comets (ROSETTA/PHILAE)

Dominique Bockelée-Morvan

Laboratoire d'études spatiales et d'instrumentation en astrophysique

Discussion 2:

Is there any limit for the molecular complexity in space? Multi-wavelength detection, and understanding the formation mechanisms

chaired by

Pierre Hily-Blant[1], Laurent Margulès[2]

[1]*Institut de Planétologie et d'Astrophysique de Grenoble*
[2]*Laboratoire de Physique des Lasers, Atomes et Molécules*

The Genesis of PCMI

Evelyne Roueff

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I will report on the early days of PCMI in the pre-IRAM era and the subsequent development of the interdisciplinary French community interested in the Physics and Chemistry of the Interstellar Medium.

The ISO [1] and Herschel [2] missions have also played a crucial role in extending the areas of PCMI to grain physics and surface chemistry.

How can we further progress? The availability of ALMA [3] data offers the opportunity to define new challenges. Preserving such an interdisciplinary environment is decisive to move forward and PCMI provides a unique frame to bridge different skills.

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[2] http://www.cosmos.esa.int/
[3] http://www.eso.org/sci/facilities/alma.html

European Task Force for Laboratory Astrophysics (ETFLA)

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The European Task Force for Laboratory Astrophysics (ETFLA) was set up by FP7 project Astronet to develop a strategy to optimize and promote the field of laboratory astrophysics. ETFLA issued a mid-term report [1] which makes a number of recommendations. These recommendations and the actions resulting from them will be ouylined at the meeting.

If you wish to be kept up to date on developments in this area you can subscribe by sending an e-mail to LISTSERV@JISCMAIL.AC.UK with the following command in the e-mail message body: SUBSCRIBE LABASTRO

References

[1] ETFLA Midterm report on recommendations regarding the establishment of a European Laboratory Astrophysics Network (Nov. 2013), available from www.labastro.eu

Laboratory Astrophysics Division of the American Astronomical Society (AAS/LAD)

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The purpose of the Laboratory Astrophysics Division (LAD) of the American Astronomical Society (AAS) is to advance our understanding of the Universe through the promotion of fundamental theoretical and experimental research into the underlying processes that drive the Cosmos. LAD represents all areas of astrophysics and planetary sciences.

The first new AAS Division in more than 30 years, the LAD was established in 2012 and traces its history back to the recommendation from the scientific community via the White Paper from the 2006 NASA-sponsored Laboratory Astrophysics Workshop. This recommendation was endorsed by the Astronomy and Astrophysics Advisory Committee (AAAC), which advises the National Science Foundation (NSF), the National Aeronautics and Space Administration (NASA), and the U.S. Department of Energy (DOE) on selected issues within the fields of astronomy and astrophysics that are of mutual interest and concern to the agencies. In January 2007, at the 209th AAS meeting, the AAS Council set up a Steering Committee to formulate Bylaws for a Working Group on Laboratory Astrophysics (WGLA). The AAS Council formally established the WGLA with a five-year mandate in May 2007, at the 210th AAS meeting.

From 2008 through 2012, the WGLA annually sponsored Meetings in-a-Meeting at the AAS Summer Meetings [2]. In May 2011, at the 218th AAS meeting, the AAS Council voted to convert the WGLA, at the end of its mandate, into a Division of the AAS and requested draft Bylaws from the Steering Committee. In January 2012, at the 219th AAS Meeting, the AAS Council formally approved the Bylaws [1] and the creation of the LAD. The inaugural gathering and its first business meeting of the LAD were held at the 220th AAS meeting in June 2012.

The operating structure of the Laboratory Astrophysics Division, the role of the Division within the AAS and its goals and objectives will be presented. You can learn more about LAD by visiting its website at http://lad.aas.org/, by subscribing to its mailing list [3] and/or by joining the LAD [4].

References:

[1] Bylaws of the Laboratory Astrophysics Division. http://lad.aas.org/business_and_bylaws
[2] Meetings of the Laboratory Astrophysics Division. http://lad.aas.org/meetings
[3] Communication, http://lad.aas.org/listserv
[4] Membership, http://lad.aas.org/members

Formation of hydroxylamine from ammonia and hydroxyl radicals.

An astrochemically-relevant two-step mechanism

Emilie-Laure Zins, Lahouari Krim

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In the interstellar medium, as well as in icy comets, ammonia may be a crucial species in the first step toward the formation of amino-acids and other prebiotic precursor such as hydroxylamine (NH_2OH). Using either electron-UV irradiations[1,2] of water-ammonia ices or successive hydrogenation[3,4] of solid nitric oxide, laboratory experiments have already shown the feasibility of reactions that may take place on the surface of ice grains in molecular clouds, and may lead to the formation of this precursor. Herein is proposed a new reaction pathway involving ammonia and hydroxyl radicals generated in a microwave discharge. Experimental studies, at 3 and 10 K, in solid phase as well as in neon matrix have shown that this reaction proceed via a hydrogen abstraction, leading to the formation of NH_2 radical, that further recombine with hydroxyl radical to form hydroxylamine, under non-energetic conditions.

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UV laser desorption time-of-flight mass spectrometry of VUV photo-processed ices

Jean-Baptiste Bossa[1], Daniel Paardekooper[1], Karoliina Isokoski[1]

and Harold Linnartz[1]

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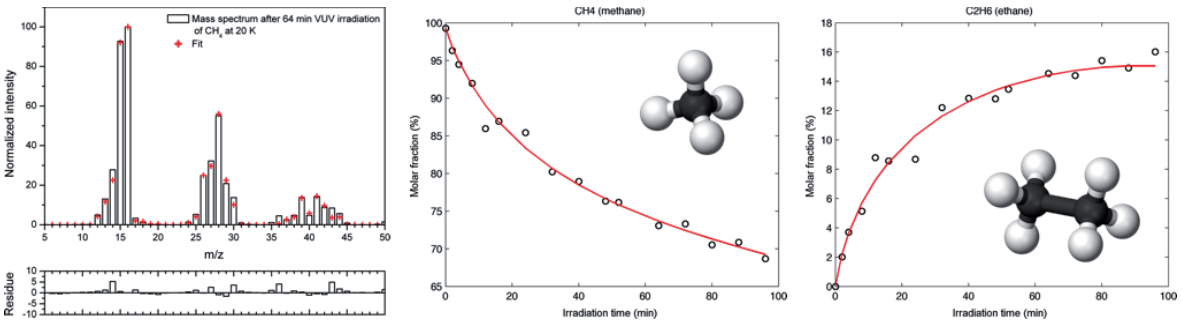
Advances in telescope and interferometer arrays have highlighted a rich and exotic chemistry occurring in the surroundings of star-forming regions, as evidenced by the detection of more than 170 molecules and ions in space. Complex organic molecules (> 6 atoms) have been unambiguously detected, but their formation mechanism and corresponding yields are still unknown. Following astronomical observations, laboratory studies and models, it has become clear that surface chemistry on icy grains steadily increases the chemical diversity and offers a way to explain the molecular complexity in space. So far, systematic experimental investigations on the formation of complex organic molecules have been restricted, mainly due to the limitations imposed by standard solid-state techniques. To overcome these limitations, a new experimental setup as been designed.

A new ultra-high vacuum experiment is described that allows studying photo-induced chemical processes in interstellar ice analogues [1]. MATRIICES: a Mass Analytical Tool to study Reactions in Interstellar ICES applies a new concept by combining UV laser desorption and time-of-flight mass spectrometry with the ultimate goal to characterize *in situ* and in real time the solid state evolution of organic compounds upon VUV photolysis for astronomically relevant ice mixtures and temperatures

The performance of the experimental setup is demonstrated by the kinetic analysis of the different photoproducts of pure methane ice at 20 K. A quantitative approach provides molar fractions at the different stages of the VUV irradiation. These data are then kinetically fitted to a reduced chemical reaction network in order to obtain the rate constants and ultimately the branching ratios of photochemical reactions yielding new species with up to four carbon atoms. Convincing evidence is found for the formation of even larger species.



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Hydrogen/deuterium exchanges in interstellar ice analogs

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Star-forming regions in the interstellar medium or small bodies in planetary systems are both known for the presence of extreme deuterium enrichment. Deuterium fractionation is mainly due to zero point energy effects in these cold environments. Nevertheless, this single process is insufficient toreproduce observations like the enrichment disparities between functional groups and other chemical mechanisms have to be considered. The hydrogen-deuterium spontaneous exchanges between water and organic molecules are studied experimentally. The aim is to provide a quantitative description of this process and to derive the corresponding rate constants for (solid-phase) astrochemical networks. Thin films of water ice mixed with a few percentof deuterated organic molecules(methylamine (CD_3ND_2) or methanol (CD_3OD)) are condensed at low temperature (< 40K) and warmed up to 140K. The chemical evolution of the film is then followed by Fourier transformed infrared spectroscopy (FTIR), as in Ratajczak et al. [1].Our work shows that rapid H-D exchanges occur in the ice duringthe crystallization process, specifically between the amine or alcohol functional groups and water. The H-D exchanges between water and methylamine are found to obeya second-order kinetics. The temperature dependence follows an Arrhenius law with an activation energy of ~ 4000K.

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Diffusion-limited reactivity in interstellar ice

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Interstellar grains are thought to play an important role in the formation of complex molecules in the interstellar medium[1]. However, the low temperature and scarcity of reactants present in their ice mantle strongly limit the formation of complex molecules. Whether or not long time scale can counterbalance this diffusion-limited solid-state reactivity at low-temperature depends on both the reaction rate constant and the diffusion coefficients of the reactants, whether they are neutrals or radicals.

I will present our combined experimental and theoretical study undertaken in order to better understand the importance of such a diffusion limited reactivity mechanism. As a model system the two reactants CO_2 and NH_3 are chosen. They are abundant in interstellar ices and have been shown to react thermally in ices[2] to give NH_2COOH and $NH_4^+NH_2COO^-$. The reaction rate constant of the NH_3 + CO_2 reaction in a water free environment is measured and the reaction mechanism rationalized on the basis of *ab-initio* calculations mimicking this reaction in both an ammonia and a water-ammonia cluster. This reaction is also studied in a more realistic water ice model using *ab-initio* molecular dynamic technics. The diffusion coefficients of CO_2 and NH_3 in the ice are determined using both laboratory experiments, classical and *ab-initio* molecular dynamics simulations. Our goal with this study is to use our determined diffusion coefficients and rate constant for the NH_3 + CO_2 reaction in a water ice model to develop a diffusion-reaction formalism to account for the slowing down induced by an increasing dilution of the reactants in the water ice mantle. The diffusion-limited reaction rate may be extrapolated to lower temperature and longer time scale to set a limit to the production of complex molecules in interstellar ice.

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Chimie des glaces :

formation des molécules complexes et photodésorption

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Les grains et les glaces interstellaires jouent un rôle important dans la formation des molécules complexes, de la formation des molécules simples pendant la transition du milieu diffus au milieu dense, à la formation de molécules complexes lors de la formation d'étoiles. Différents processus, sur la surface ou dans le manteau des glaces, thermiques ou non-thermiques, sont responsables de cette évolution chimique.

Dans cette contribution, je passerai en revue les différents travaux en laboratoire qui ont pour but de reproduire les processus interstellaires à l'œuvre dans la phase solide: le chauffage thermique, la photochimie, le bombardement par des particules chargées, ainsi que la désorption thermique, la désorption chimique ou la photodésorption. Bien que ses travaux expérimentaux aient largement amélioré notre compréhension de la chimie interstellaire en phase solide, la quantification des différents processus est un défi de premier ordre en astrophysique de laboratoire.

Interstellar grains and interstellar ices play an important role in the formation of complex molecules, from the formation of simple molecules during the diffuse to dense transition of a cloud, to the formation of complex molecules during star formation. Different processes, both on the surface and in the mantle of the ice, involving both thermal and non-thermal processes, are responsible of this chemical evolution.

In this talk, I will review different laboratory works aiming at mimicking the interstellar processes at work in the solid state: thermal heating, photochemistry, charged particles bombardment as well as thermal, chemical or photo- desorption. Although these experimental works brought important progresses in the understanding we have in solid-state interstellar chemistry, the quantification of the different processes is a key challenge in laboratory astrophysics.

Bright CO clumps resulting from the interaction of the HD34078 runaway star with the diffuse IC405 nebula

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Some runaway stars are known to display IR arc-like structures around them, resulting from their interaction with surrounding interstellar material. The properties of these features as well as the processes involved in their formation are still poorly understood.

We obtained and analyzed a high spatial resolution map of the CO(1-0) emission that is centered on the runaway O star AEAur (HD34078), and that combines data from both the IRAM interferometer and 30m single-dish antenna. The line of sight towards HD34078 intersects the outer part of one of the detected globulettes, which accounts for both the properties of diffuse UV light observed in the field and the numerous molecular absorption lines detected in HD34078's spectra, including those from highly excited H2. These globulettes have a high density and linewidth, and are strongly pressure-confined or transient. (Gratier et al. 2014)

Wide-field imaging of this region with the IRAM-30m telescope reveals about 25 bright ($\sim$ 10K) and small ($< 22''$) CO clumps, while no CO emission is detected in the low angular resolution (>15') CO surveys (the classical Dame et al. (2001) and the latest Planck maps). The majority of these clumps are located on the parabolic interface that has been shaped by the star - ISM interaction. Measures of Halpha extinction combined with scattered blue light show that the bright CO clumps correspond to translucent gas with a typical extinction of Av$\sim$2–5. Most of these clumps have detected CN emission which favors quite dense gas (nH2 = 1e4-1e6 cm-3) for such an overall diffuse environment. We will present recent work resulting from on-going 5"-resolution, large mosaic (163 fields) observations with the PdBI. These observations should enable us to answer the questions concerning the origin and fate of these bright CO clumps, which exists while illuminated by an intense UV radiation field of HD34078 (χ = 100 − 10000 depending on the star-clump distance).

High spatial resolution observations of key hydrocarbon species in the NGC 7023 PDR

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Carbon is an important building block of both interstellar gas and dust in Photo-Dissociation Regions (PDRs). A significant fraction of carbon (up to 20%) is tied up in the carriers of the Aromatic Infrared Bands (AIB), which consist in Polycyclic Aromatic Hydrocarbons (PAH) and evaporating very small grains (eVSG) [1,2]. The nature of PAHs and eVSGs and their link with smaller hydrocarbons are still under debate, in particular their aliphatic/aromatic composition [3,4] and whether their photo-destruction can inject fresh hydrocarbons into the gas phase, which could explain why the abundances of small hydrocarbons (e.g., CCH and c-C_3H_2) in cool PDRs are one order of magnitudes higher than those predicted by current gas-phase chemical models [5].

In this contribution, we study the aromatic-aliphatic nature of PAH-related molecules and their link with gas phase chemistry by analyzing IR and radio observations of the NGC 7023 PDR at high angular resolution: the mid-IR Spitzer data allows us to study the evolution of the AIB carriers under the action of UV photons; AKARI near-IR observations provide information on the aromatic and aliphatic nature of PAHs and eVSGs; finally, mm-wave data obtained with the Plateau de Bure Interferometer and with the IRAM 30m telescope are used to investigate the chemical link of these species with gas-phase species CCH and c-C_3H_2.

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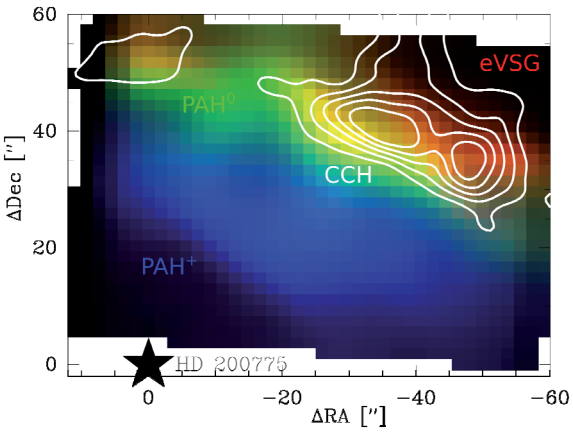

Figure 1: The NW PDR of NGC 7023 decomposed in PAH^+ (blue), PAH^0 (green) and eVSGs (red). Contours represent the integrated intensity of the CCH N=1-0 line (steps of 0.25K km s^{-1}).

Impact of ionization compression on turbulent molecular clouds, and dating of OB associations.

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The expansion of hot ionized gas from an Hii region into a turbulent molecular cloud compresses the material and leads to the formation of dense continuous layers as well as pillars and globules in the interaction zone. This feedback should also impact the probability distribution function (PDF) of the column density around the ionized gas. We aim to quantify this effect and investigate its link to the Initial Mass Function (IMF) using Herschel column density maps and 3D simulations with the HERACLES code. The double-peaked/enlarged shape of the PDF in high-mass star-forming regions could impact the gravo-turbulent scenario used to derive the CMF supposed to be at the origin of the IMF [1].

We derived also an analytical solution that follows the expansion of the region in a turbulent medium and test is against 1D and 3D simulations. From the corresponding 1D simulations, we computed a grid of models that can be used to estimate the age of large sample of OB associations. We applied the method to the HRDS survey and tested it on well-known regions. This method could also be used for the dating of extra-galactic Hii regions [2].

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Environmental impacts of the irradiated shocks in the W28 A2 massive star-forming region

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The formation of massive stars plays a crucial role in the interstellar medium of galaxies from numerous points of view. They are a critical source of energy and momentum input: they send shock waves propagating in their environment through their ejection structures (jets and bipolar outflows), and the energetic radiation field emitted by the central object is likely to cause dissociation and ionization in its surroundings. In this talk, I will illustrate the propagation of so-called 'irradiated shocks' in the W28 A2 star-forming region, corresponding to outflows that are illuminated by the radiation field of the forming proto-star. I will present observations from the APEX, Herschel, and IRAM 30m telescopes, and use them to characterize the chemical (carbon-bearing species: CO, C, C^+, CH^+, but also SiO) and energetic (mass, energy, momentum, ejection rates) impact of such outflows. Additionnally, in W28 A2, strong fluxes of high-energy photons have been detected by the gamma-ray telescopes HESS and Fermi, hinting at the presence of energetic cosmic rays in the region. I will show to which extent our precise sub-mm dataset can provide a contribution to the study of their possible origin in W28 A2, in relation with the presence of the strong shocks powered by the massive forming star.

Dynamical properties of warm and dense photodissociation regions: from the interstellar medium to protoplanetary disks

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The surface layers of molecular clouds and protoplanetary disks harbor photodissociation regions (PDRs) where neutral gas is heated by the ultraviolet photons (UV) of nearby stars. The balance between heating mechanisms (mainly photo-electric heating, and heating by H2 de-excitation and formation), and cooling in far-infrared lines (mainly [CII] and [OI] fine structure lines), determines the structure of PDRs and therefore of a large fraction of the interstellar medium. While the thermal balance of PDRs has been largely investigated in the past, and now with Herschel, little is known about the dynamical properties of PDRs. Here we present spatially and spectrally resolved HIFI maps of the [CII], 12CO(8-7) and 13CO(8-7) emission of two prototypical PDRs: the NGC 7023 and Horsehead nebulae, which allow us to study gas kinematics in PDRs. The analysis, using blind signal separation algorithms, of the [CII] maps and comparison to the molecular lines indicates that these PDRs are dynamically active. In particular, we find evidence (especially in NGC 7023) that photo-evaporation is occurring. This process can have a significant impact on the density and thermal structure of highly irradiated PDRs and perhaps play a role in triggered star-formation. In addition, the detection of photo-evaporation flows in extended PDRs of star-forming regions offers the possibility to study this mechanism in details, as a template for photo-evaporation in protoplanetary disks. I will also briefly present the recent results obtained with Herschel (see J. Champion et al., this conference) for a protoplanetary disk in the Carina nebula where external irradiation is suspected to ignite photo-evaporation. We used the techniques developed for extended PDRs to interpret the observations of high-J CO, [CII] and [OI] lines in this source, and found that the surface of this disk is indeed at very high pressure and therefore unstable against photoevaporation. However, we found that the mass-loss rate through photoevaporation is limited, either by gravitational forces or magnetic fields.

The JWST project: Applications to PDRs or shocks

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The James Webb Space Telescope (JWST) should be launched in 2018, with a 6.5-meter primary mirror and four imaging and spectroscopic (R=100-3000) instruments working from 0.6 to 28.5 microns. The PCMI community must be prepared to use this unique facility whose access will be open but strongly competitive**.** First call for Proposals should be issued approximately 1 year before launch.

I will present the expected performances of the instruments. The gain in angular resolution and sensitivity will be at least one order of magnitude compared to previous infrared observatories.With an angular resolution better than 1 arcsec (or 0.002 pc/400 UA for a distance of 400 pc), it will be possible to resolve the spatial scales in nearby galactic objects (photodissociation regions – PDRs, shocks, disks, …)where key physical processes are acting. Illustrative examples will be presented.

Discussion 3:

Star formation yields, 3D structure of the ISM: The role of magnetic field, turbulence, stellar feedback and cosmic rays

chaired by

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X-ray observations of supernova remnants and the future European X-ray observatory Athena

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I will present a review of X-ray observations of supernova remnants in the era of XMM-Newton and Chandra satellites. These observations provide a wealth of information both on the enriched hot ionized plasma ejected by the supernova, and on the particles accelerated at the main shock in the surrounding interstellar medium, constraining the supernova evolution and particle acceleration at their shock.

I will then introduce the future European X-ray observatory, Athena, L2 mission of the ESA cosmic vision programme, to be launched in 2028.

Dust temperature fluctuations and surface chemistry: H_2 formation.

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Among dust grains, very small grains and PAHs are known to be of dominating importance for various processes. Indeed, big grains contain most of the dust mass, but the smallest grains dominate the total dust surface. Small grains are thus also the principal substrate for surface reactions, the most important of which is the formation of H_2.

However, models of H_2 formation must take dust temperature fluctuations into account. Small grains are sensitive to individual UV photons and undergo temperature spikes. Yet surface chemistry models almost always assume a non-fluctuating grain temperature. While this assumption is reasonable for the surface chemistry in dark cloud cores, it is much less justified for H_2 formation in UV-rich environments (e.g., diffuse gas or bright PDRs).

Various mechanisms can contribute to H_2 formation. The Langmuir-Hinshelwood mechanism involves physisorbed atoms migrating on the surface, and was experimentally found to have a limited temperature range of efficiency (10-20K) [1], while ISO and Spitzer observations of PDRs show efficient formation despite warmer dust [2]. Other mechanisms were proposed such as the Eley-Rideal mechanism [3], involving direct reaction between a chemisorbed atom and a gas atom, and insensitive to grain temperature.

We present the first complete analytical treatment of the statistical problem of surface chemistry with fluctuating temperatures, using a master equation approach to follow exactly both the temperature and the population of adsorbed atoms. We apply this treatment to the Langmuir-Hinshelwood mechanism and find it to be much more efficient than expected in unshielded environments under moderate UV fields, as the grain spends most of its time at temperatures lower than its average temperature. Another mechanism is still necessary to account for formation under strong UV fields, and the Eley-Rideal mechanism is found to retain most of its efficiency. Fast approximations of the exact results are constructed.

The effects of this new formalism on full cloud simulations are explored using the Meudon PDR code [4]. Effects are found in tracers of the cloud edge (H_2, CH^+) but remain limited. The increase in Langmuir-Hinshelwood efficiency nevertheless allows more flexibility in the choice of the poorly known microphysical parameters of the Eley-Rideal mechanism, as will be demonstrated using the constraints of the observations of a few well-known PDRs.

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Probing the impact of metallicity on the dust properties in galaxies

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As galaxies evolve, their Interstellar Medium (ISM) becomes continually enriched with metals, and this metal enrichment influences the subsequent star formation. Low-metallicity dwarf galaxies of the local Universe are ideal candidates to study the influence of this metal enrichment on the ISM properties of galaxies. Previous studies have shown that the ISM of dwarf galaxies poses a number of interesting puzzles in terms of the abundance of dust grains, the dust composition and even the FIR emission processes. Before the advent of Herschel, these studies were limited to the warmer dust emitting at wavelengths shorter than 200 microns and were done only on a small number of dwarf galaxies. Thanks to its increased sensitivity and resolution in FIR and submillimeter (submm) wavelengths, *Herschel* gives us a new view on the cold dust properties in galaxies and enables us to study the lowest metallicity galaxies in a systematic way.

We carried out a systematic study of the integrated dust properties in a sample of ~110 local Universe galaxies, using the dust continuum spanning the near-infrared to millimetre wavelengths and realistic dust models, and compared this to the gas properties. We considered two Herschel surveys (the Dwarf Galaxy Survey and the KINGFISH sample; [1,2]) spanning a wide range of galactic properties in terms of metallicity, but also morphological type, stellar mass, star formation activity, etc.

Our study reveals different dust properties in low-metallicity environments compared to those observed in more metal-rich systems (e.g., an overall warmer dust component) [3,4], which will be presented here. An excess submm emission is often apparent near and/or beyond 500 microns rendering large uncertainties in the dust properties, even for something as fundamental as dust masses. We will discuss the appearance of this submm excess in our sample and test alternative dust composition, with more emissive grains, to explain this excess emission [3,4]. Ideal tracer of the chemical evolutionary stage of a galaxy, the gas-to-dust mass ratios (G/D) is found to be much higher than what is expected by simple chemical evolution models. We will then focus on the relation between G/D and metallicity and interpret it with the aid of different chemical evolution models to explain this unexpected trend [5].

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What does the study of nearby galaxies teaches us about the ISM processes?

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It is much more common to think about "how our knowledge of interstellar medium (ISM) processes from the lab or from detailed studies in our Galaxy impacts what we know about nearby galaxies" than the reverse. This is mainly due to the idea of going from high to low resolution, going from individual regions to integrated ones, etc.

However, the increase in resolution of infrared to millimeter observations and the rise of very large surveys in the optical and radio domain give us the possibility to study the ISM of nearby galaxies with more and more precision. Furthermore, nearby galaxies enable us to sample a wider range of environments, for example in metallicity. Also, studying different regions within a nearby galaxy is a unique opportunity to be free of the effect of distance and to get an outsider view (no -or fewer- confusion along the line of sight), two uncertainties that are making studies in our Galaxy more difficult. Finally, if the galaxy is observed with enough resolution and fully covered, one can get a global picture of all the ISM phases in a galaxy. Studies of nearby galaxies hence bring important clues on different processes at stake in the interstellar medium.

I will review different studies of nearby galaxies, with some bias toward the Magellanic Clouds since these galaxies are the easiest to observe due to their proximity and location on the sky. In particular, I will touch upon the evolution with metallicity of the structure of molecular clouds and their interface, dust mass budgets, molecular clouds/star formation evolutionary sequences, ...

H_2 Formation

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H2 is the most abundant molecule in the Universe, observed in a large variety of environments from the cold Interstellar Medium to the early Universe. Its formation still poses unresolved physical problems, coming mainly from its homonuclear character.

After reviewing its main structural properties, I will present what is (thought to be) known on its formation in the Solar neighborhood, how these processes are modified in less and less metallic environments (where dust abundances are reduced) [1], and eventually in neutral primordial gas before formation of the first starts [2].

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Water formation through O_2+D pathway on cold silicates and amorphous water surfaces of interstellar interest

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Interstellar water formation has been intensively investigated in the past decade. Many studies from different groups have shown an efficient formation through the hydrogenation/deuteration of O atoms, O_2 and O_3 ices [1-3], mostly in the multilayer regime [1,2]. We present the first experimental results for D_2O and D_2O_2 molecules formation through O_2 +D pathway in the sub-and monolayer regimes on bare amorphous silicate grain analogs. For comparison, we investigated water formation on porous and non-porous amorphous solid water ices surfaces held at 10 K [4]. The experiments were performed with the FORMOLISM setup using atomic deuterium and molecular oxygen triply differential pumping beam lines. We covered the surface of the sample with one monolayer of solid O_2 at 10 K and we irradiated the film with D-atoms at the same surface temperature until the destruction of the oxygen species. The gas surface reactions were analyzed with Reflection Absorption Infra-Red Spectroscopy (RAIRS) and Temperature-Programmed Desorption (TPD) techniques.

Results showed that the formation of D_2O water molecules is very efficient through the O_2+D pathway, but one fraction of the newly formed water stays on the dust grains at 10 K, and the other fraction is released into the gas phase. The fraction of water molecules desorbing into the gas phase upon formation depends strongly on the substrate (silicate or water ice). In the case of the silicates, about 90 % of the newly formed D_2O water molecules are released into the gas phase by chemical desorption process [5]. The non-thermal desorption of D_2O water products results from the high exothermicity of the OD+D $\rightarrow$ D_2O reaction [6]. These results are supported by a kinetic chemical model taking into account the high desorption rate of water products.

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Formation of molecules at the gas-surface interface: experimental and theoretical advances

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In the interstellar medium, dust grains catalyze the formation of molecules. In order to understand and quantitatively describe such processes, it is necessary to study the interactions (and reactions) of H, C, O atoms from interstellar clouds with (and at) grain surfaces, and the dynamics of molecular formation of H_2, OH, H_2O, etc.

Molecules can be formed from two atoms which are adsorbed on a dust grain (Langmuir-Hinshelwood mechanism), from one adsorbed atom and an atom from the gas phase (Eley-Rideal mechanism), or by a mixture of these two mechanisms.

In this talk, I will present theoretical and experimental studies of the formation of H_2 and OH molecules on dust grains. Theoretically, the structure of dust grains can be modelled using electronic structure calculations or analytical potentials, and is then used for simulating the dynamics of the reactions. This leads to the calculation of physical quantities such as cross section of reactions, ro-vibrational excitations, and energy repartitions between molecules and dust grains.

Small scale structure of IRC+10216 : a key to time dependent chemistry.

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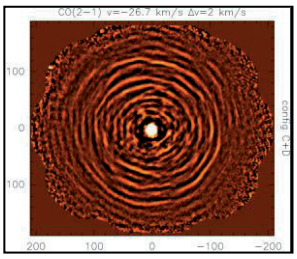
IRC+10216/CW Leo is the closest high mass loss AGB star (D ≃ 130 pc). It is surrounded by a spherical envelope with an exceptionally rich molecular content. Over 80 molecular species have been detected in this envelope, which have largely contributed to our understanding of circumstellar (CS) and interstellar (IS) chemistry. IRC+10216's outer envelope expands radially at a nearly uniform velocity (14. 5 km/s, or 1'' per 50 years). This remarkable property and the envelope large angular size make it a unique probe of time-dependant chemistry over timescales of thousands of years.



Using the SMA, PdBI and the IRAM30-m telescope, we have investigated the structure of IRC+10216 at angular resolutions of 1'' to 30''. We have studied the spatial distributions of a score of molecular species (C-chains, metal compounds, anions,..) as well as that of the molecular gas. The latter is best traced by the CO line emission, up to the CO photodissociation radius R_{phot}~ 180''. It yields a lookup time ≃ 10^4 yr on the mass-loss process. The CO map (synthetized beam 3'') reveals a spectacular pattern of thin spherical shells atop a broad centrally peaked pedestal (Fig. 1). It teaches us about the clumpiness of the gas, the presence of shocks and the penetration of the IS radiation inside the envelope – three powerful boosters of CS and IS chemistry. We will present the first results of our investigation by focusing on their implications for the radical and anion chemistry.

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Hydrogenated Amorphous Carbons: evolution of interstellar carbon dust

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Observations of infrared (IR) bands (emission and absorption) show that polycyclic aromatic hydrocarbons (PAH) and hydrogenated amorphous carbons (HAC or a-C:H) are both important component of interstellar carbon matter, as macromolecules and solid dust particles, respectively. The main IR absorption feature of a-C:H dust (at 3.4 μm) has been first detected in diffuse interstellar medium toward the Galactic center in the early eighties [1]. Now, several IR bands are widely observed, also in external galaxies [2], showing the ubiquitous nature of interstellar a-C:H dust component. Their observables and properties will be reviewed.

A important issue concerns the evolution of a-C:H in the different astrophysical environments and how it is related to the cycle of matter in a galaxy. Exposition to UV photons, energetic particles such as those of cosmic rays, shocks, hydrogen atoms,or thermal annealing can alter the structure and properties of this hydrocarbon dust, and thus induce a modification of the corresponding observables. I will present results that have been obtained on this topic from observations, models, and laboratory experiments.

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The Formation of Solid Particles from their Gas-Phase Molecular Precursors in Cosmic Environments

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We present and discuss the characteristics and capabilities of the laboratory facility, COSmIC, that was developed at NASA Ames to generate, process and analyze interstellar, circumstellar and planetary analogs in the laboratory [1]. COSmIC stands for Cosmic Simulation Chamber and is dedicated to the study of molecules and ions under the low temperature and high vacuum conditions that are required to simulate interstellar, circumstellar and planetary physical environments in space. COSmIC integrates a variety of state-of-the-art instruments that allow forming, processing and monitoring simulated space conditions for planetary, circumstellar and interstellar materials in the laboratory [2]. COSmIC is composed of a Pulsed Discharge Nozzle (PDN) expansion that generates a free jet supersonic expansion coupled to two high-sensitivity, complementary in situ diagnostics: a Cavity Ring Down Spectroscopy (CRDS) system for photonic detection and a Reflectron Time-Of-Flight Mass Spectrometer (ReTOF-MS) for mass detection. Recent laboratory astrophysics results that were obtained using the capabilities of COSmIC will be discussed, in particular the progress that has been achieved in monitoring in the laboratory the formation of solid gains from their gas-phase molecular precursors with applications that extend to environments as varied as stellar/circumstellar outflows [3] and planetary atmospheres [4]. Plans for future, next generation, laboratory experiments on cosmic molecules and grains in the growing field of laboratory astrophysics will also be addressed as well as the implications of the current studies for astrophysics.

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PAHs from circumstellar environments to the interstellar medium. The Nanocosmos project

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Polycyclic aromatic hydrocarbon (PAH) molecules are the best carriers for the strong aromatic IR bands (AIBs) at 3.3, 6.2, 7.7, 8.6, 11.3 and 12.7 microns that are observed in emission in many astronomical environments where UV photons are available. It has been shown that these UV photons not only trigger the AIB emission but also play a role in the chemical production of the band carriers. In photodissociation regions associated to star formation, a scenario has been proposed in which gas-phase PAHs are produced by photoevaporation of very small grains, which could be PAH clusters ([1] and references therein). In evolved stars, which are the major sites of dust formation in our Galaxy, PAH emission is only observed when the central star emits strongly in the UV, which happens while the object evolves from the AGB to the planetary nebula (PN) phase. The evolution of the IR spectrum suggests that UV-processing induces the destruction of fragile aliphatic bonds and the formation of a more aromatic material that is likely the precursor of PAHs [2].

The Nanocosmos ERC Synergy project aims at investigating the physical and chemical conditions that lead to complex hydrocarbon chemistry and ultimately to the formation of PAHs and other large carbonaceous molecules such as C_{60}. Observations are planned with ALMA for prototype stars in transition between the AGB and PN phases, in order to understand whether the formation of large hydrocarbons is spatially associated with the dense torus as well as the role of radical-radical reactions versus ion-molecule reactions. In the laboratory, we will investigate various chemical routes to form PAHs and related species involving both gas-phase and gas-grain interactions. For instance, recent studies have suggested the role of crystalline silicates [3] or SiC grains [4] in the formation of PAHs. Our laboratory studies will take benefit from setups and reactors already in operation in Toulouse and in Spain. They will also involve the development of new simulation chambers. Studying the processing of the formed species by UV photons (which often requires access to synchroton VUV beamlines) as well as recording their IR spectroscopy in cosmic conditions are also key aspects of the project.

The Nanocosmos ERC Synergy project (2014-2020) is led by the three PIs: J. Cernicharo and J. A. Martín-Gago (ICMM, CSIC, Madrid) and C. Joblin (IRAP, CNRS, Toulouse). Several research teams and institutes are involved on both sides. In Toulouse, IRAP, LCAR, LCPQ and LAPLACE laboratories carry the activity.

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Discussion 4:

Nucleation, coagulation, clustering processes, photolysis, formation and desorption of ices. Impact on ISM and protoplanetary disks

chaired by

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Cosmic-ray induced ionization of a molecular cloud shocked by the W28 supernova remnant

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Cosmic rays are an essential ingredient in the evolution of the interstellar medium, as they dominate the ionization of the dense molecular gas, where stars and planets form. However, since they are efficiently scattered by the galactic magnetic fields, many questions remain open, such as where exactly they are accelerated, what is their original energy spectrum and how they propagate into molecular clouds. In this work, we present new observations and discuss in detail a method that allows us to measure the cosmic ray ionization rate towards the molecular clouds close to the W28 supernova remnant. To do so, we use CO, HCO+ and DCO+ millimeter line observations and compare them with the predictions of non-LTE radiative transfer and chemical models. The CO observations allow us to constrain the density, temperature and column density towards each observed position, while the DCO+/HCO+ abundance ratios provide us with constraints on the electron fraction and, consequently, on the cosmic ray ionization rate. Towards positions located close to the supernova remnant, we find cosmic ray ionization rates much larger (> 100) than that in standard galactic clouds. Conversely, towards one position situated at a larger distance, we derive a standard cosmic ray ionization rate. Overall, these observations support the hypothesis that the γ-rays observed in the region have an hadronic origin. In addition, based on CR diffusion estimates, we find that the ionization of the gas is likely due to 0.1 – 1 GeV cosmic rays. Finally, these observations are also in agreement with the global picture of cosmic ray diffusion, in which the low-energy tail of the cosmic ray population diffuses at smaller distances than the high-energy counterpart.

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The flux of cosmic rays and the physical conditions in the Central Molecular Zone of our Galaxy inferred by H_3^+

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The Central Molecular Zone (CMZ) is the region spanning over 200 pc around the central Black Hole of our galaxy, Sgr A*. The nature and physical conditions of this area has been a long subject of debate. H_3^+ has been detected on more than 10 lines of sight in this region [1]. These detections are surprising and characteristic of very specific processes taking place in our Galaxy Center. First, H_3^+ has column densities 10 times higher in the CMZ than in typical diffuse interstellar clouds. Second, it is detected in its (3,3) metastable level that is not observed elsewhere. This indicates that a large fraction of the Central Molecular Zone of our Galaxy must be filled with diffuse neutral gas (< 500 cm-3) and that mechanisms heat this gas at about ~400 K (whereas standard diffuse clouds, heated by photo-electric effect, have a temperature of 60 K).

Several authors, of the ISM community, but also of the high energy astrophysics community, tried to infer the physical conditions in the CMZ. Most of these studies are based on H_3^+ observations or on tracers of cosmic rays as the synchrotron emission from the CMZ [2]. In these works, the large abundance of H_3^+ is explained by an intense flux of cosmic rays, about 10-100 times higher in the CMZ than in typical diffuse clouds. Nevertheless, no consistent explanation has been proposed to explain both, the large abundance of H_3^+ and its unusual excitation / temperature of the gas. The most common proposition is to assume that shocks or turbulence could be an important source of heating that would excite H_3^+.

In this talk, we will present a comprehensive model of the physical conditions and processes in the Central Molecular Zone of our Galaxy. This model has been obtained with the new version of the Meudon PDR code [3] in which recent H_3^+ + H_2 collision rates [4] have been implemented. We will first show that the column density of H_3^+ is not proportional to the flux of cosmic rays under the exotic conditions of the CMZ (on the opposite to classical ISM). We will then show that a detailed treatment of the physics of grains and PAHs - that control H_2 formation and electrons recombination - has a strong influence on the abundance of H_3^+. On the opposite to classical models, thanks to detailed treatment of the physical processes, we find for the first time a scenario that explains both the abundance of H_3^+ and its unusual excitation. It it then possible to better constrain the properties of the CMZ. We will show, that this scenario is also compatible with the conclusions of specialists of high energy astrophysics studying the CMZ with synchrotron emission.

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SO5 - Plateforme MIS & Jets

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Un réel retour scientifique des grands instruments (ALMA, IRAM/Noema, Herschel, …) ne sera possible que si la communauté a accès à des codes de référence pour interpréter leurs données. En 2012, l'INSU a labellisé le service SO5 « Plateforme MIS & Jets » [1] dont l'objectif est de fournir un ensemble d'outils théoriques basés sur des codes de référence (PDR, Choc Paris-Durham, TDR, RAMSES-MHD) pour faciliter la préparation et l'interprétation des observations dans le gaz moléculaire galactique et extragalactique.

Plusieurs services sont déjà fonctionnels: accès aux codes, à des simulations numériques lourdes de coeurs pré-stellaires (champs de densité, champ de vitesse, …) et à des grilles de modèles PDR pour des régions de formation d'étoiles (intensité de raies, densités de colonne des espèces …)[2][3].

Afin de faciliter d'avantage la confrontation modèles - observations, une seconde génération de services est en cours de développement. En effet, les services les plus attendus par la communauté sont 1) la fouille de modèles, i.e. un outil permettant d'identifier parmi une grille de modèles pré-calculés ceux vérifiant un jeu de contraintes observationnelles, 2) un service de lancement de codes avec ressources de calcul en ligne. De tels services représentent un défi à la limite de la R&D informatique puisqu'il s'agit de manipuler des centaines de milliers voire des millions de méta-données très rapidement - chose impossible avec des technologies classiques de bases de données.

Dans cet exposé, nous présenterons les services disponibles: base de données PDR, code de choc Paris-Durham en ligne, Starformat, ainsi que le prototype de datamining. Nous présenterons la stratégie de développement pour les prochaines années (simulateur ALMA, base de données de chocs MHD, …). Enfin, nous présenterons le pôle thématique national SO5 qui se met en place à la demande de PCMI et de l'INSU pour coordonner ce type de services. Au cours de l'exposé, nous montrerons comment des technologies informatiques de pointe peuvent être utilisées pour développer des services novateurs.

PCMI étant le programme national le plus concerné par le service SO5 « Plateforme MIS & Jets », l'un des objectifs de cette présentation est aussi de recueillir des avis de la communauté pour préciser la stratégie de développements de nos services.

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Attempts at characterizing the structures of high dissipation in the interstellar medium.

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Regardless of the mechanisms which stir the interstellar gas, the damping of its turbulent motions must occur at much smaller scales, where microscopic dissipative processes such as viscous friction, Ohmic resistivity or ambipolar diffusion can take place. The resulting heating is therefore likely to be extremely localised and intense, thus highly susceptible to open new chemical routes. The chemical species produced in the wake of such hot spots should therefore help us to study observationnally the turbulent dissipation mechanisms in the interstellar gas.

We first present 3D magnetohydrodynamic simulations (with ambipolar diffusion) of decaying turbulence in which we extract the structures of high dissipation. We show that these structures are highly coherent and that their geometrical properties obey remarkable statistical scalings. We present attempts at characterizing their location in the plane of the sky through maps of centroid line velocities or polarisation angle increments.

We then examine small scale 2D hydrodynamic simulations (with chemistry) of decaying turbulence. In this 2D set up, highly dissipative structures are along ridges and we observe a strong molecular enhancement in their wake. We fit steady-shocks locally to these structures and we examine the statistics of their entrance parameters. We finally examine how much these shocks can account for the average chemical abundances in our simulations, to estimate when other forms of dissipation (such as shearing sheets / vortices) are needed or not.

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3D interstellar chemo-physical evolution (3DICE)

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Carbon and heavier atoms are born in the centre of stars. At the end of their life, stars spread their inner material into the diffuse interstellar medium. This diffuse medium gets locally denser and form dark clouds (also called dense or molecular clouds) whose innermost part is shielded from the external UV field by the dust, allowing for molecules to grow and get more complex. Gravitational collapse occurs inside these dense clouds, forming protostars and their surrounding disks, and eventually planetary systems like (or unlike) our solar system. The formation and evolution of molecules, minerals, ices and organics from the diffuse medium to planetary bodies, their alteration or preservation throughout this cosmic chemical history set the initial conditions for building planets, atmospheres and possibly the first bricks of life.

The evolution of the gas and dust chemical composition during this sequence is a continuous process in the sense that the chemical composition never reaches steady-state. The chemical composition in one of the steps then depends on the previous ones. The current view of interstellar chemistry is, however, based on fragmental works on key steps of the sequence that are observed. Astrochemists develop models to study the chemical composition of dense clouds, protostars or protoplanetary disks assuming the initial condition from the previous step and use the physical conditions observed in the present objects.

The objective of this project, funded by an ERC Starting Grant, is to follow the fractionation of the elements between the gas-phase and the interstellar grains, from the most diffuse medium to protoplanetary disks, in order to constrain the chemical composition of the material in which planets are formed. The potential outcome of this project is to get a consistent and more accurate description of the chemical evolution of interstellar matter.

What do we learn from surveys (GAIA, Pan-STARRS, VISTA, etc) concerning the structure and phases of the ISM (3D ISM, extinction curve and diffuse bands studies)

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The solution for the dark night sky paradox suggested by Olbers (1823) is actually the first mention of a non-transparent Interstellar Medium (ISM). The paradox is solved by extinction (which we know now is wrong!). Extinction is a fundamental property of the ISM which is basically observed from short wavelengths to the mid-infrared. In my talk I discuss the impact of the large surveys that produce star catalogues with accurate photometry on the ISM studies. They allow the mapping of the extinction independently of the dust grain temperature fluctuations, which contaminate the column density maps derived from dust thermal emission; these star catalogues also make it possible to constrain the extinction law. When the distances of the stars are known, the third dimension of the ISM structure can be investigated. Hipparcos, in the early 90's, was not accurate enough for such analysis but a wealth of new data is arriving with surveys such as Pan-STARRS and Gaia. The 3D extinction measurement from these surveys, combined with the submm/mm emission will obviously help us to understand the ISM better.

Visible and near-infrared spectroscopy of interstellar matter with ground-based instruments.

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Spectroscopy of interstellar matter at visible and infrared wavelengths remains an important tool for investigating chemical evolution, both in our Galaxy and in diffuse gas at high redshift. I will review recent developments that point the way toward future studies. High-resolution infrared spectroscopy of interstellar H_3^+ provides direct information about the rate of cosmic-ray ionizations. This can now be complemented by near-UV observations of OH^+, which probes molecular gas of low molecular fraction. The recent observation of CH^+ in an external starburst galaxy, M82, may lead to a better understanding of turbulent dissipation. Measurements of isotope abundances of the light elements (D/H, ^{6}Li/^{7}Li, ^{10}B/^{11}B) are now possible in external galaxies, with implications for our understanding of cosmic evolution. The UV/visible afterglows of gamma-ray bursts provide background light sources for sensitive absorption spectroscopy to study interstellar matter in host galaxies at high redshift. The chemistry and physics of disks around young stellar objects can be studied advantageously through near-infrared spectroscopy. A sensitive, high-resolution spectropolarimeter like SPIRou will make it possible to investigate circumstellar envelopes and planet-forming disks in new ways.

What is the status of the current models of our Galaxy?

Frédéric Bournaud

Institut de recherche sur les lois fondamentales de l'Univers

Discussion 5:

How to model the physics/chemistry of ISM (1D PDR, 1D shock, 3D MHD, 3D radiation transfer,...). Impact of the accuracy limitations and predictive capability of models?

chaired by

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Présentation par affiche

Présentation par affiche
Poster n° 1

Water clusters embedded in a rare gas matrix : anharmonic IR spectra from MD simulations using a hybrid SCC-DFTB/FF method

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A part of our activities has recently been dedicated to the theoretical studies of water clusters, isolated and adsorbed on polycyclic aromatic hydrocarbons (PAHs) [1]. The electronic structure is described with the Self-Consistent-Charge Density Functional based Tight Binding (SCC-DFTB) method [2], very efficient (faster than exact DFT approaches) to treat very large systems. Describing the electronic structure at the SCC-DFTB level allows to perform on-the-fly Born Oppenheimer molecular dynamics (BOMD) simulations within a reasonable timescale, aiming at approaching the statistical behaviour of such large and floppy systems as water clusters adsorbed on PAHs. Using this approach, we determined the influence of the PAH surface on the isomerisation reactions and IR spectra of small water clusters $(H_2O)_n$ (n=2-8).

We now aim at describing such clusters embedded in a rare gas (Ar) matrix, in the context of our collaboration with the group of J. Mascetti (ISM, Université Bordeaux I, ANR PARCS 13-BS08-0005-02) where experiments in cryogenic environment are carried out. We have recently developed a hybrid SCC-DFTB/Force Field (SCC-DFTB/FF) scheme to describe the interactions of water-PAH clusters with rare gas atoms, thus allowing the explicit dynamics of the matrix. This model was benchmarked on the structures and energetics of $(C_6H_6)^{0/+}Ar_n$ clusters [3]. We then investigated the influence of the Ar matrix on the structural, energetic, dynamic and spectroscopic properties of water clusters $(H_2O)_n$ (n=1-6) with BOMD simulations using the SCC-DFTB/FF potential. The embedded single water molecule was shown to rotate at 13±1K, in line with experimental data. The IR bands (H_2O stretching modes) were shown to be redshifted with respect to isolated H_2O, with the redshift values in line with experimental results. Results for larger clusters, in particular for the interesting case of the water hexamer (the smallest 3 D structure) that presents several low-lying isomers, will also be presented.

Future studies will concern water-PAH clusters and inclusion of nuclear quantum effects with the Path Integral Molecular Dynamics approach.

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Présentation par affiche
Poster n° 2

Complex Organic Molecule formation: grain surface or gas-phase chemistry?

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Complex organic molecules (COMs) have long been observed in the warm regions of star forming regions surrounding nascent protostars, first in massive hot cores, and later in their low-mass counterparts. The large richness in chemical species displayed in the spectra of these regions has triggered the development of chemical models aiming at accounting for the observed chemical complexity. It was first proposed that simple molecules like e.g. methanol were injected into the gas phase when the icy mantles were evaporated during the protostellar phase. These species could then react in the gas via ion-molecule reactions followed by dissociative recombination to form COMs. Later experimental and theoretical work has however shown that these gas-phase processes were unable to produce sufficient amounts of COMs as observed. Alternative COM formation mechanisms were proposed in which atoms or diatomic molecules (e.g. CO, N) were hydrogenated on the grains during the pre-stellar phase. Heavy radicals formed on the grains can diffuse during the warm-up phase when the ice temperature reaches ~ 30 K to form COMs, which are subsequently released in the gas phase at higher temperatures. The recent discovery of COMs like methyl formate or dimethyl ether in pre-stellar cores [1], where gas and dust temperatures rarely exceed 10-15 K, casts doubt on this type of scenario, as the ice is never warm enough to enable the diffusion of radicals necessary to the formation of complex species. The question of COM formation has therefore to be investigated again: do non-thermal processes play a role in increasing radical mobility or should new gas-phase routes be explored?

The radicals involved in the formation of the aforementioned COMs, HCO and CH_3O represent intermediate species in the grain-surface synthesis of methanol which proceeds via successive hydrogenation of CO molecules in the ice (gas-phase synthesis of methanol is believed to be inefficient). Detection of COMs in another cold source, including the radical CH_3O and the similar abundances found for these species has led to the speculation that they were probably formed on the grain surfaces. We present here observations of methanol and its precursors HCO, H_2CO, CH_3O in a sample of pre-stellar cores and derive their relative abundances. We find that the relative abundances are constant across the core sample. Our results also show that the amounts of HCO and CH_3O are consistent with a gas-phase synthesis of these species from H_2CO and CH_3OH via radical-neutral or ion-molecule reactions followed by dissociative recombination. Thus, while grain chemistry is necessary to explain the abundances of the "parent" volatiles CH_3OH and H_2CO, the reactive species HCO and CH_3O might be "daughter" molecules directly produced in the gas-phase.

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Présentation par affiche
Poster n° 3

A combined Experimental and Theoretical Kinetic study of reactions between a series of alkylamines with CN radicals at 23 to 300 K

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The search for the origins of life and its presence beyond Earth is a matter of concern for all the humanity especially the scientific community which seeks for precursor molecules of amino acids (bricks of DNA and RNA). It is then important to identify the different formation and destruction processes of these molecules in the conditions of extraterrestrial media.

Among these, methylamine (CH_3NH_2) which has been discovered in the interstellar media (Sgr B2 and Ori A) since 1974 [1], can be the terminal product of a series of hydrogenation of HCN: $HCN \xrightarrow{H} CH_2NH \xrightarrow{H} CH_2NH_2 \xrightarrow{H} CH_3NH_2$. Once formed, the substitution of one of its hydrogen atom by a carboxyl group (COOH) can lead to the formation of the glycine (the simplest amino-acid) in the interstellar media.

Astrophysical and astrobiological interest of this molecule led us to undertake a gas phase kinetic study of a series of alkyamines: methylamine CH_3NH_2, Dimethylamine $(CH_3)_2NH$ and Trimethylamine $(CH_3)_3N$ in the presence of the CN radical in interstellar conditions at temperatures ranging from 24 K to 300 K using the CRESU technique (Cinétique de Réaction en Ecoulement Supersonique Uniforme / Reaction Kinetics in a Uniform Supersonic Expansion). This technique generates a low temperature flow reactor via isentropic expansion of a gas through a convergent-divergent Laval nozzle producing a radially and axially uniform supersonic flow at a given temperature, density and velocity. In order to determine the rate coefficient of the reaction of alkylamines with the CN radical, the CRESU apparatus was coupled to Pulsed Laser photolysis (PLP) and Laser Induced Fluorescence (LIF) techniques. The rate coefficients of the studied reactions were determined from the temporal evolution of the fluorescence signal as a function of the alkylamines concentrations. The reactivity of alkylamines with CN is found to be very fast and the measured rate coefficients are close to the collisional rates ($4\text{-}5\times10^{-10}$ $cm^3molec.^{-1}s^{-1}$). For dimethylamine and trimethylamine no temperature dependence was observed whereas, methylamine presents a slight negative temperature dependence.

Additionally, a theoretical study is in progress in order to determine the products and the branching ratios of the possible pathways for the reaction of CN with methylamine.

Présentation par affiche
Poster n° 4

Photodesorption of interstellar ices: role of indirect processes and of photochemistry

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In cold regions of the Interstellar Medium (ISM), like star-forming regions or protoplanetary disks, molecules form or accrete on the surface of dust grains. The resulting icy mantles represent the main reservoir of molecules beside H_2. At the very low temperatures of these regions, thermal processes can be neglected, but energetic processes, for instance induced by cosmic rays or photon impact on the ices, can promote their desorption and therefore enrich the gas phase with cold molecular species. In particular, it is at present known that the desorption induced by UV photons – the UV photodesorption – is an efficient process. The photodesorption rates are considered in several different regions of the ISM in order to explain abundances of molecules in the gas phase [1,2].

These last years, we have developed a new experimental approach for the study of the UV photodesorption from simple model ices, using the brilliance and the accordability of synchrotron radiation from the DESIRS beamline at the SOLEIL facility. The studies, resolved in the energy of the incident photons, allows for the determination of absolute energy-dependent photodesorption rates that can be applied to any interstellar-relevant UV field. Moreover, the method gives valuable information on the underlying molecular mechanisms in the ice, highlighting the crucial role played by the composition of the ice on the overall photodesorption efficiency [3].

Using this approach, we have identified that the photodesorption from simple ices is mainly driven by an indirect process: the energy absorbed by a molecule is redistributed in its close-surrounding, leading the ejection of another, surface-located species. In some other cases, the photodissociation of condensed molecules plays also an important role, and can even become the dominating desorption pathway. In this presentation, I will illustrate these different cases by presenting results obtained on pure and mixed ices of non-dissociating molecules N_2 and CO, and on ices of CO_2.

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Présentation par affiche
Poster n° 5

Ethylene Glycol detection in Orion KL: fighting spectral confusion by classical and by new statistical methods

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Despite a good first order correlation between chemical abundances in comets and hot cores[1], complex oxygenated species do show differences. Ethylene glycol $(CH_2OH)_2$ has been difficult to detect in the Galactic center source Sgr B2 (Hollis et al 2002)[2], but has proven relatively more abundant in comets (Crovisier et al 2004a, Biver et al 2014)[3,4]. Its companion molecule, glycolaldehyde CH_2OHCHO, shows similar abundances in Sgr B2, while it is not detected in our Orion-KL PdBI data (Favre et al 2011)[5] and only a five times lower limit has been obtained in comet C/1995 O1 (Hale-Bopp)[6]. Similarly, ethanol, CH_3CH_2OH, an abundant species in the interstellar medium, is not yet detected in comets. These molecules appear thus as key species in the comparison of interstellar and cometary ices, and the subsequent discussion on the formation of cometary matter.

We focus here on ethylene glycol and present its first detection in the nearest and best studied hot core-like region, Orion-KL (Brouillet et al, submitted)[7]. Whereas we got first hints of the presence of this molecule as early as 2004 in IRAM PdBI data, it is only now that we think we can claim a reliable detection. The main reason for that is the high level of spectral confusion in the very rich Orion-KL spectra.

We present first the analysis of ALMA Science Verification Orion data which lead to this detection, the necessary steps we performed to fight the effect of spectral confusion - where maps and a large bandwidth (34GHz) played a very important role - and the procedure we used to subtract carefully the continuum emission.

We discuss then the first results of an on-going study aimed at handling the problem of spectral confusion by developing dedicated statistical tools, which are tested within the R software.

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Présentation par affiche
Poster n° 6

Origin and excitation mechanisms of the warm CO, OH and CH^+ in PDRs

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Photon Dominated Regions (PDRs), where physics and chemistry are driven by FUV photons, show an extremely rich and warm photochemistry that is closely related to that of protoplanetary disks and starburst galaxies. The rotationally excited lines of CO, OH and CH^+ probe the warmest PDR gas layers, providing strong constraints for understanding the physics and chemistry in strongly FUV-irradiated interstellar clouds. The far-IR OH and high-J CO emission lines have been associated with the presence of unresolved dense structures and high pressure gas [e.g., 1, 2, 3]. For CH^+, highly reactive, excitation is driven by collisions and by chemical pumping after reaction of C^+ with vibrationally excited H_2 [4, 5].

For the first time we present fully sampled PACS maps (110" x 110") of the CO J=19-18, OH 84 and 119 μm and CH^+ J=3-2 lines in the Orion Bar. The spatial distribution of these lines confirms the clumpy structure of the Bar and constrains the origin of high-J CO, OH, and CH^+ to the dense clumps. Excitation mostly occurs at the PDR edge, where the UV flux is at maximum in the PDR. Photoelectric effect on small particles is the dominant heating source of the observed high excited molecular gas and the effect of cosmic rays is excluded. It is clear that the vibrationally excited H_2 is the key in the formation and excitation of CH^+. To a lesser extent, excited H_2 is also relevant for OH formation. Interestingly, the peak OH emission corresponds with a bright young object identified as a proplyd, which confirms that this line is tracing dense irradiated structures [6]. Using the spectral and spatial distribution of several CO lines and its isotopes, we present temperature and column density maps over this area covering the entire Orion Bar. We estimate the thermal pressure and the size of the small irradiated dense structures. This study strongly supports the high pressure PDR model of Joblin et al. [3].

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Présentation par affiche
Poster n° 7

Random mixtures of polycyclic aromatic hydrocarbon spectra match interstellar infrared emission

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The mid-infrared (mid-IR; 5–15 μm) spectrum of a wide variety of astronomical objects exhibits a set of broad emission features at 6.2, 7.7, 8.6, 11.3, and 12.7 μm. About 30 years ago it was proposed that these signatures are due to emission from a family of UV heated nanometer-sized carbonaceous molecules known as polycyclic aromatic hydrocarbons (PAHs), causing them to be referred to as aromatic IR bands (AIBs). Today, the acceptance of the PAH model is far from settled, as the identification of a single PAH in space has not yet been successful, and physically relevant theoretical models involving «true» PAH cross sections do not reproduce the AIBs in detail. Using the NASA Ames PAH IR Spectroscopic Database [1,2], which contains over 500 quantum-computed spectra, in conjunction with a simple emission model, we found that the spectrum produced by any random mixture of at least 30 PAHs converges to the same «kernel-spectrum» (Fig. 1). This kernel-spectrum captures the essence of the PAH emission spectrum and is highly correlated with observations of AIBs (Fig. 1), strongly supporting PAHs as their source. The fact that a large number of molecules are required implies that spectroscopic signatures of the individual PAHs contributing to the AIBs, spanning the visible, near-IR, and far-IR spectral regions are weak, perhaps explaining why they have not yet been detected so far. An improved effort, joining laboratory, theoretical, and observational studies of the PAH emission process is needed to help achieving a specific identification and support the use of PAH features as a probe of physical and chemical conditions in the near and distant Universe.

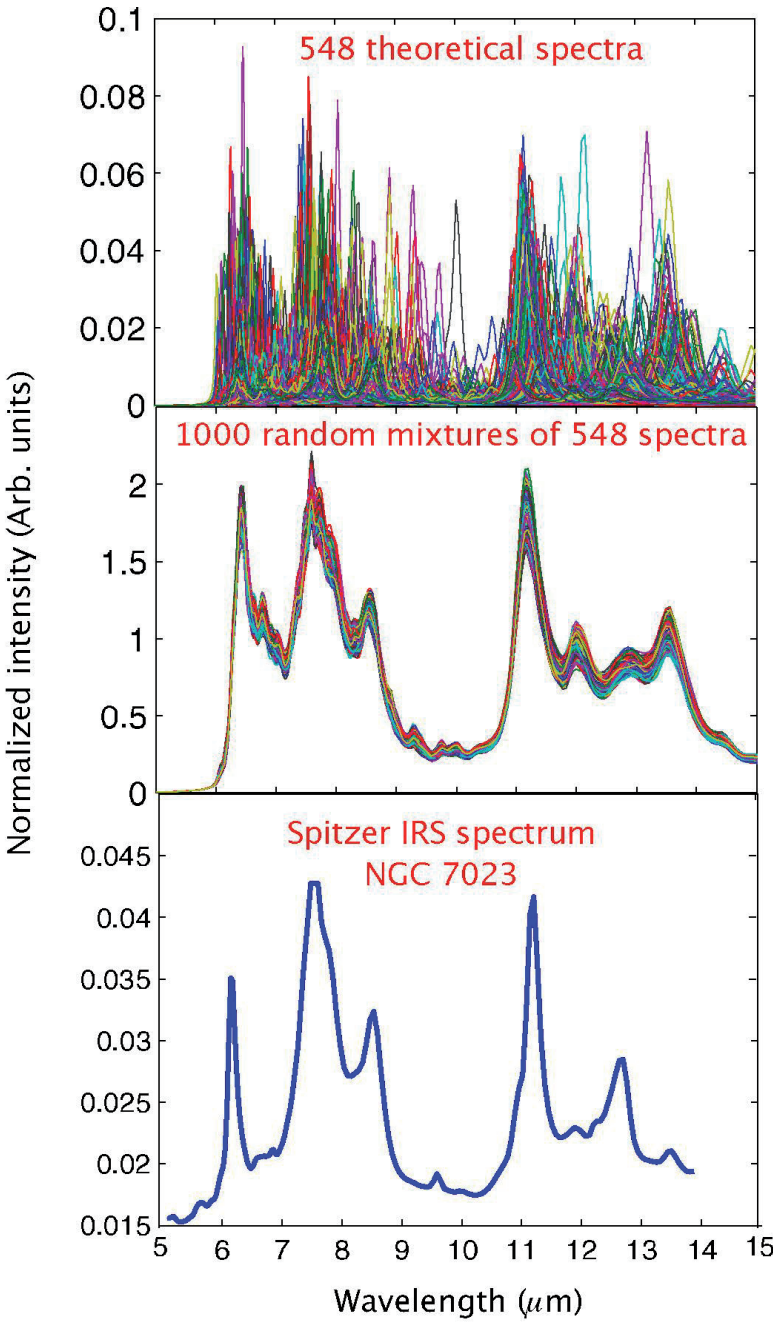

Figure 1 - Upper: 548 theoretical spectra of PAHs from the NASA Ames Spectroscopic database. Middle: 1000 mixtures of the 548 theoretical spectra using random weight coefficients, illustrating how all the mixtures appear identical. Bottom: Observed spectrum of the NGC 7023 reflection nebula. Adapted from [3]

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Présentation par affiche
Poster n° 8

Complex Organic molecules in the cold envelope of the solar type protostar IRAS16293-2422

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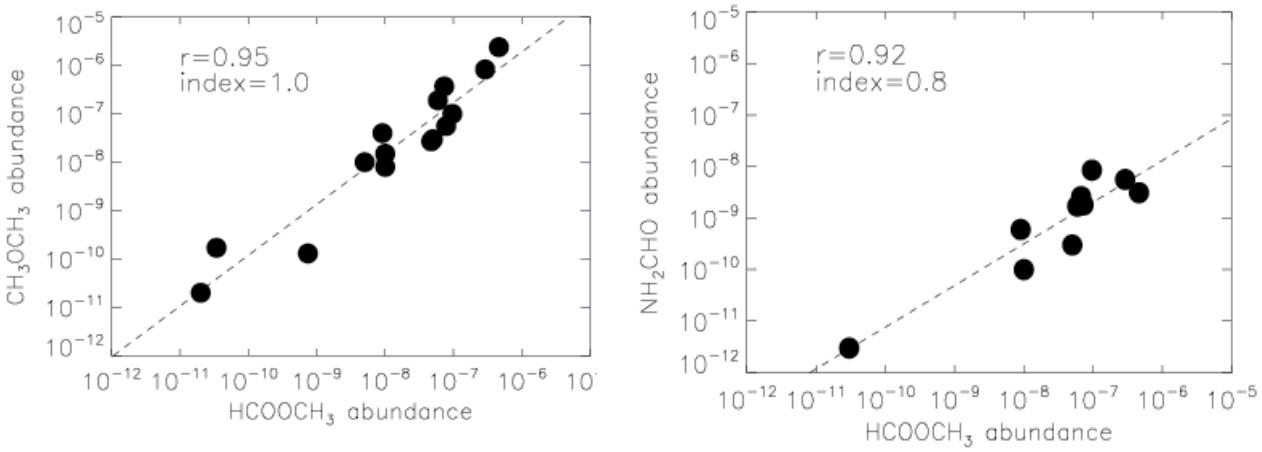
Complex Organic Molecules (COMs) are considered crucial molecules, since they are connected with organic chemistry, at the basis of the terrestrial life. These molecules are a crucial test for astrochemical models. Current models assume that several COMs are synthesised on the lukewarm grain surfaces (30-40 K), and released in the gas phase at dust temperatures >100 K. However, recent detections of COMs in < 20 K gas demonstrate that we still need important pieces to complete the puzzle of the COMs formation. We present here the analysis of five oxygen and nitrogen bearing COMs towards the solar type protostar IRAS16293-2422, obtained from the millimeter-submillimeter unbiased spectral survey TIMASSS [1] : ketene, acetaldehyde, formamide, dimethyl ether, and methyl formate. These COMs are present in the cold (< 30 K) envelope of IRAS16293-2422 and their abundances do not increase with increasing dust temperature in the cold envelope, as expected if COMs were predominately formed on the lukewarm grain surfaces [2]. When considering also other ISM sources, we find a strong correlation (see Fig. 1) between the methyl formate and dimethyl ether and methyl formate and formamide abundances, which may point to a link between these two couples of species, in cold and warm gas.

A similar core – envelope analysis is being performed on cyanopolyynes and their isotopes. The results, in terms of molecule and isotopic ratios distribution in the hot corino and its cold envelope will also be presented.

Fig:1 Abundance of dimethyl ether (left), formamide (right) as a function of the abundance of methyl formate in different ISM sources.



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Présentation par affiche
Poster n° 9

Gas-phase ion-molecule chemistry: an experimental study of $CH_3^+ + CH_4$ and $C_{2p+1}N^- + HC_3N$ (p=0-1)

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Together with the heterogeneous chemistry occurring at the surface of dust grains, gas-phase ion-molecule chemistry is of great importance to account for the chemical complexity observed in the interstellar medium. Yet, understanding the abundance and excitation of some species like CH^+ remains a major challenge and the recent discovery of anionic species ($C_{2p}H^-$; $C_{2p+1}N^-$) points out the need for new chemical networks.

In this contribution, we will present recent results concerning both *(i)* the reactivity of the CH_3^+ ion with CH_4 as a function of CH_3^+ internal excitation and *(ii)* the reactions of the CN^- and C_3N^- ions with HC_3N.

(i) Although the reactivity of the methyl cation with hydrocarbons has been widely studied in the past, here we report on experiments where the CH_3^+ ion is generated *via* direct photoionization of the CH_3· radical. This allows for the production of the ion within a controlled degree of internal excitation, thus opening the possibility to investigate the effect of internal degrees of freedom (vibrational, electronic) on the reactivity.
Branching ratios and absolute reaction cross-sections have been obtained for the $CH_3^+ + CH_4$ reactive system. Reaction dynamics and dependence on the vibrational excitation of the parent ion will be discussed.

(ii) Experimental investigations of ion-molecule reactions involving small $C_{2p+1}N^-$ ions have been undertaken in a common effort between several French and Czech groups [1-4]. Here we will present new measurements at 300K obtained in Orsay using a FT-ICR spectrometer for the following reactions: $CN^- + HC_3N$; $C_3N^- + HC_3N$; $C_3N^- + HC_3{}^{15}N$; $C_3{}^{15}N^- + HC_3N$.
Kinetic rate constants have been determined and several mechanisms including fast proton transfer and slower associative detachment have been identified and will be discussed [4].

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Présentation par affiche
Poster n° 10

The WHISPER line survey (Wideband High resolution IRAM 30m Survey at two Positions with EMIR Receivers) : complex organics in the horsehead UV illuminted edge

V. V. Guzman[1], P. Gratier[2] , J. Pety[3], M. Gerin[4], J.R. Goicoechea[5], E. Roueff[4], F. Le Petit[4], J. Le Bourlot[4].

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This poster summarizes our recent results on the ISM physics and chemistry in the Horsehead nebula, from a complete and unbiased line survey performed with the IRAM-30m telescope, where approximatively 30 species (plus their isotopologues) are detected with up to 7 atoms. The detections obtained with this survey illustrate the interplay between the solid and gas phase chemistry in the formation of (complex) organic species like H_2CO, CH_3OH and CH_3CN, and confirm that photo-desorption by FUV photons is an efficient mechanism to release frozen species in the gas phase [1,2,3]. The case of CH_3CN is especially surprising as it is 40 times more abundant in the warm UV-illuminated edge of the nebula than in the cool well shielded core. Other complex molecules such as HCOOH, CH_2CO, CH_3CHO and CH_3CCH are also detected in the PDR [4]. The hydrocarbon ion C_3H^+, identified in the ISM thanks to this survey [5] has recently been confirmed by laboratory experiments [6]. High angular resolution observations have now been obtained with the plateau de Bure interferometer confirming its association with the FUV illuminated region.

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Présentation par affiche
Poster n° 11

Molecular abundances in the gas phase: how much do they depend on differential adsorption at interstellar surfaces? The CHON isomers as a case study.

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The CHON generic chemical formula covers four different isomers, isocyanic acid (HNCO), cyanic acid (HOCN), fulminic acid (HCNO) and isofulminic acid (HONC), the first three being identified in a large variety of interstellar environments. The knowledge of their relative abundance ratios with respect to the most stable one is a crucial data for constraining astrochemical models. For most of the species observed so far in the interstellar medium (ISM), the most abundant isomer of a given generic chemical formula is the most stable one (*minimum energy principle – MEP*). The few exceptions have been linked to different pathways of formation and destruction involving gas phase and/or surface processes that may be thought different according to the local temperature and the nature of the support (water ice, carbonaceous matter, silicate …).

In order to project some light on the interaction of the CHON isomers with interstellar grains as a function of the nature of their surfaces and determine how these surfaces may influence the observed abundances, we employed the means of numerical simulations. Using first principle periodic density functional theory (DFT) to represent the interacting support as a solid of infinite dimension, the adsorption energies were calculated on hexagonal ice, on graphene and on quartz.

It was found that, whatever the nature of the surface, there were two different classes of isomers; one weakly bound (HNCO and HCNO) and one strongly bound (HOCN and HONC) with a ratio ~ ½ in adsorption energies. We have also shown that it is the hydrogen bonding which plays the discriminating role in the trapping of CHON species on grains surfaces.
The adsorption energies are in the order HOCN > HONC > HNCO > HCNO and are totally disconnected from the relative stabilities HNCO >HOCN >HCNO > HONC of the CHON isomers.
Whatever the environment, differential adsorption is effective and its contribution to the molecular abundances observed cannot be ignored.

Présentation par affiche
Poster n° 12

The survival of PAHs and hydrocarbon nanoparticles in H II regions

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Observations show that emission from the Unidentified Infrared (UIR)bands is strongly suppressed in H II regions. UIR bands are generally attributed to vibrational relaxation of FUV -excited Polycyclic Aromatic Hydrocarbon (PAH) molecules (e.g., [1]) or hydrocarbon nanoparticles containing aromatic domains (e.g., [2]). If the strongly reduced UIR emission in H II regions has to be ascribed to the suppression of the carriers, an efficient destruction mechanism needs to be found in order to explain observations. Our previous work [3] has shown that collisional dissociation induced by ions and electrons is not effective in H II regions. On the other hand, various studies (e.g., [4, 5]) have shown that small PAHs (< 50 carbon atoms) are quickly destroyed by UV photons.

In this study, we model the photo-processing of large PAHs (> 50 carbon atoms) and hydrocarbon nanoparticles of similar size under a set of physical conditions representative of well studied H II regions. This allows us to clarify whether processing by UV photons is indeed responsible for the observed lack of infrared emission.

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Présentation par affiche
Poster n° 13

Toward complex nitrile molecules in astrophysical environments: low temperature kinetic study of C_3N^- with cyanoacetylene HC_3N

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Almost 30 nitrile molecules, which contain the cyano group (C≡N), have been detected in the interstellar medium (ISM) so far. The simplest of these nitriles, the cyano radical C≡N, was found in 1940[1,2]. The most complex of all nitriles, $HC_{11}N$, having a total of 13 atoms, was detected in 1997[3]. The complexity of the ISM was further confirmed with the recent identification of six molecular anions: C_4H^-, C_6H^-, C_8H^-, CN^-, C_3N^-, and C_5N^-[4]. The most prolific source of anions discovered to date is the envelope around the carbon-rich evolved star IRC +10216. This object is the only source where all six anions have been identified, even though anions are also observed in prestellar and protostellar clouds. These charged species have a large reactivity and seem to play a key role for the formation of complex nitriles as it was shown recently in some models including reactions involving nitrile anions [5,6]. However, our understanding of anion-molecule reactions (kinetics and branching ratios) of potential interest for planetary sciences and astrophysics remains very limited. So far, less than ten laboratory studies have investigated the temperature dependence of the rate coefficients of reactions involving anion reactants below 200 K.

We present here a kinetic exploration between 300 and 50 K of the gas phase reaction of the C_3N^- anion with cyanoacetylene HC_3N. Cyanoacetylene has been detected in various astrophysical environments such as IRC+10216 [7], SgrB2 [8], TMC-1[9] as well as in the atmosphere of Titan. The products of the reaction and the temperature dependence of the rate coefficient have been studied using the CRESU method coupled with mass spectrometry which is well adapted to study in the gas phase ion-neutral reactions under the low temperatures prevailing in cold astrophysical environments.

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Présentation par affiche
Poster n° 14

REACTIONS OF NEUTRAL PAHs IN CRYOGENIC SOLIDS

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Polycyclic aromatic hydrocarbons (PAHs) are good candidates for AIBs (aromatic interstellar bands), assigned to vibration modes of PAHs, which emit in the infrared (IR) between 3 and 20 μm after absorption of star UV light, and for DIBs (diffuse interstellar bands), which are weak absorption bands measured in the visible range between 0.38 and 1.3 μm. However, no specific PAH has been identified yet, and a variety of PAH-derived species (ionized, substituted, coordinated) have been proposed. The aim of our work is to bring new elements for the understanding of these assignments through the study of:

1) Reactions of PAHs with Fe atoms and aggregates. The hypothesis of the formation of metal complexes $Fe_x(PAH)_y$ is proposed to account for the depletion of Fe from the gaseous phase of the interstellar medium.

2) Photo-reactions of PAHs in water ice. In dense molecular clouds, atoms and molecules are condensed on cold dust and ice particles, where they are transformed by thermal and photochemical processes. UV-visible and FTIR spectroscopies, associated to matrix isolation techniques, are the main tools used to study the composition of interstellar ices. We have recently proposed IR identification of quinones, alcohols and ketones through photo-irradiation of coronene andpyrene embedded in amorphous solid water (1).

Our study proposes joint theoretical and experimental treatments of these reactions in order to understand how these molecules are formed.In the theoretical part, we describe the dynamic processes that drive these reactions in the environment (matrix, ice). The reaction products and mechanisms are characterized through their vibrational (IR) and electronic (UV-visible) spectra. IR spectra are derived from molecular dynamics simulationswith the electronic structure determined with methods derived from Density Functional based Tight Binding (DFTB) (2-4). In particular, ahybrid DFTB/Force Fieldapproach has been developed to take into account the matrix environment (4,5), and further development will be undertaken to describe the interaction of PAHs with water ices. Time-Dependent DFTB and wavefunction approaches will be usedto characterize the excited states and determine electronic spectra.

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Présentation par affiche
Poster n° 15

The chemistry of interstellar ices in the laboratory: the case of amino acids

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An understanding of the chemical reactions occurring within interstellar grains provides insights on the level of complexity of the molecules that can be expected to exist within asteroids or comets. The study of potential chemical pathways towards the formation of amino acids or their precursors on these grains is of great interest to astrochemistry. Indeed, once interstellar grains agglomerated to form bodies such as comets, they were able to bring to Earth the organic matter necessary for the development of a prebiotic chemistry.

The Strecker reaction is a chemical pathways leading to the formation of amino acids, and at least some of the steps of this reaction are conceivable within interstellar ices. Thanks to an experimental setup allowing us to study the chemical evolution of an interstellar ice analogue during its warming, we were able to validate several steps of this reaction [1, 2, 3]. Furthermore, our experiments highlighted a major role of water (the main constituent of comets) -- its ability to trap reactants in the solid phase above their respective desorption temperatures, consequently enabling reactions with higher activation energies to proceed [4].

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Présentation par affiche
Poster n° 16

Gas phase reaction of OH radicals with CH_3OH at temperatures of the interstellar molecular clouds

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Gas-phase chemical models are used by astrochemists to explain the syntheses of the observed molecules and their abundance in the interstellar medium (ISM). Rate coefficients (k) for the chemical reactions in these models should be well known. In many cases, k is an estimate value (or assumed equal to k(298 K)) or extrapolated from high temperature laboratory studies which underestimates quite often its value. Therefore, it is very important to accurately measure the temperature dependence of k for reactions of astrochemical interest in the T-range of dense molecular clouds in ISM (10-100 K). Reaction of OH radicals (first detected by Dieter et al. in 1963) with neutral molecules, such as CH_3OH (one of the most abundant molecules), are of special interest [1,2]. Here, we present the first kinetic study of the reaction of OH with CH_3OH in the temperature range 23 - 61 K using a CRESU (Cinétique de Réaction en Ecoulement Supersonique Uniforme / Reaction Kinetics using a Uniform Supersonic Expansion) device coupled to pulsed laser photolysis and laser induced fluorescence of OH techniques. The low temperatures were achieved by uniform supersonic gas expansion in a recently built pulsed Laval nozzle apparatus [3].

Rate coefficients $k(T)$ for reaction (1)

$$OH + CH_3OH \rightarrow \text{Products} \qquad (1)$$

were recently determined by Shannon *et al.* [4] and Gómez-Martín *et al.* [5] between 63 and 85 K and 56-202 K, respectively. Shannon *et al.* [4] predicted that k(~20 K) is expected to be near the gas kinetic collision limit (~10^{-10} cm^3 $molecule^{-1}$ s^{-1}). Our results indicate that the rate coefficient k at 23 K is not as fast as expected ($(4.1\pm0.9)\times10^{-11}$ cm^3 $molecule^{-1}$ s^{-1}). Preliminary results at 61 K, k = $(1.6\pm0.2)\times10^{-11}$ cm^3 $molecule^{-1}$ s^{-1}, indicate that below 100 K, k does not dramatically change. This new result will certainly improve the chemical astrophysical models.

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Présentation par affiche
Poster n° 17

Hypersonic expansion of hot gases probed by cavity ring-down spectroscopy

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Asymptotic Giant Branch stars play a major role in the formation and dissemination of complex molecules in the Interstellar Medium. These evolved stars exhibit a rich high temperature chemistry which is still not fully understood. The periodic instabilities coming from the internal shells of the star lead to an intense loss of mass towards the interstellar medium, forming a huge circumstellar envelope (CSE) around the star. Undergoing an intense radiation pressure, the dust grains formed inside the intermediate layersof the CSE contribute to drive out the matter from the star. The formation routes of these dust grains are still debated.

In Rennes, we have developed a new experimental setup mimicking the physical conditions encountered in the CSE. Our objective is to investigate the formation processes of PAHs molecules up to carbonaceous particles of nanometric size. A mixture of acetylene and hydrogen will be first heated up to 2000K – a typical temperature of the photosphere of AGB stars – and partly dissociated by pyrolysis, before to be expanded in a vacuum chamber. The resulting hypersonic expansion reproduces, at the laboratory scale, the strong supersonic winds and shock waves structure characterizing the CSE. During the expansion, the drop in temperature will initiate a recombination of the dissociation products of acetylene leading to aromatic molecules (PAHs), whose formation was already evidenced in one of our previous works[1]. Further downstream in the expansion, the temperature drop will initiate the nucleation of even larger species. We aim at probing the different formation steps of the aromatic molecules and nanometric carbonaceous particles taking place along the gas expansion by using anewly implemented ultra-sensitive Cavity Ring-Down Spectrometer (CRDS) in the infrared spectral range (1.5 – 1.7 microns). Our new experimental set-up is now operational and its performances will be highlighted with some preliminary results.

[1] ***Characterization of circumstellar carbonaceous dust analogues produced by pyrolysis of acetylene in a porous graphite reactor.*** **L. Biennier, R. Georges, V. Chandrasekaran, B. Rowe, T. Bataille, V. Jayaram, K.P.J. Reddy, E. Arunan. Carbon 47 , 3295-3305 (2009)**

Présentation par affiche
Poster n° 18

Modeling Complex Organic Molecules in dense cores: Eley-Rideal and surface complexation mechanisms

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Complex Organic Molecules (COMs) have recently been detected in the cold pre stellar core L1689b [1] and in the cold dense core B1-b [2]. From these detections, new challenges arise for current chemical models [1]. Indeed, due to the extremely low temperature in such regions, the standard picture for the formation of COMs seems no longer valid.

Recently, Vasyunin&Herbst[3] have proposed that these complex species are formed via gas phase ion-molecular and neutral-neutral chemistry from precursors such as formaldehyde and methanol. In this scenario, these precursors are formed on icy grains surfaces due to the surface mobility of light atoms. These precursors are then released in the gas-phase via efficient reactive desorption. However, the reactive desorption mechanism is not a fully understood process and it efficiency may not be as high as previously thought [4].

In this poster, we will present new surface processes that strongly modify the molecular abundances predicted by current gas-grain models. We will show how these mechanisms can help to explain the formation of COMs under cold and dense conditions. For that, we compare the observational results with our predictions using the chemical model Nautilus [5,6].

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Présentation par affiche
Poster n° 19

Photoionisation du coronene froid et de ses agrégats en phase gazeuse : résonances d'autoionisation du monomère au trimère, structure électronique du cation monomère

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Les molécules aromatiques polycliques (PAHs) sont des espèces-clés trouvées dans des environnements variés, tels que le Milieu Interstellaire, et dans les milieux de combustion. L'étude de leur spectroscopie UV et de leur photodynamique, qu'elles soient sous forme neutre ou cationique, est importante pour connaître leur structure, leurs mécanismes de formation et leur réactivité. Cette affiche présente les résultats d'une étude expérimentale du PAH prototype qu'est le coronene $C_{24}H_{12}$, et de ses petits agrégats $(C_{24}H_{12})_n$, au sein d'un faisceau moléculaire capable de fournir ces espèces isolées et froides, en utilisant le rayonnement VUV du Synchrotron SOLEIL auprès de la ligne DESIRS.

Les spectres de photoélectrons de seuil (TPES) et de rendement d'ions (TIY), résolus en masse grâce à la technique de coïncidences photoélectron-photoion, ont été obtenus et analysés en détail. Ils révèlent de façon inattendue des séries de résonances d'autoionisation intenses pour n=1, 2 et 3, présentant notamment des états de Rydberg des espèces neutres.

Une analyse précise de la structure électronique du cation monomère a été réalisée entre le seuil d'ionisation à 7.31 eV et 11,6 eV, en relation avec les spectres de photoélectrons [1] et les rares études existantes de la photoabsorption du cation [2]. La région du seuil a fait l'objet d'une modélisation théorique, qui fait apparaître le besoin d'un traitement explicite de l'interaction Jahn-Teller dans l'état fondamental D_0 du cation.

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Présentation par affiche
Poster n° 20

Photoelectron spectroscopy of HC_3N with synchrotron radiation and VUV laser, towards high resolution

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HC_3N is the smallest molecule of the $HC_{2n+1}N$ family and this species has been detected in the interstellar medium [1] and in the atmosphere of Titan [2]. Its interaction with the Vacuum-Ultraviolet (VUV) solar radiation leads in particular to ionization. The HC_3N^+ cation participates to the complex chemistry of these media but its spectroscopic characterization was still incomplete until recently.

In order to study in detail the vibronic structure of the cyanoacetylene cation, threshold photoelectron- and pulsed-field ionization photoelectron- spectroscopies were employed using SOLEIL synchrotron radiation and pulsed VUV lasers from the CLUPS laser center, respectively. These techniques allowed to assess new information such as the spin-orbit coupling constant or the accurate ionization energies. The experimental results were supported by *ab initio* calculations [3].

In the present poster, these two experimental techniques and their related results will be compared. The need for high resolution studies will be discussed and highlighted. In this framework, our current project of building the first high-resolution tunable VUV laser source in France will be presented.

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Présentation par affiche
Poster n° 21

Cross-matching of diffuse interstellar bands and radio emission data cubes: a new tool for the Milky Way large scale structure

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We show examples of diffuse interstellar band (DIB) extractions from VLT-GIRAFFE stellar spectra, focusing on targets distributed in distance in several fields. DIB strengths and Doppler shifts are obtained based on multi-component absorption models and stellar synthetic spectra specifically computed for each target. Their combination with spectrophotometric extinction/distance estimates allows to locate the DIBs along the sightlines, and to follow the evolution with distance of their radial velocites. The comparison of those velocities with HI/CO emission spectra allows to assign distances to the emitting clouds and reveals the spiral velocity/distance structure. Future parallax and DIB measurements with Gaia are expected to amplify considerably the potential outcome of such analyses.

Présentation par affiche
Poster n° 22

Photodissociation of gas-phase PAH cations in interstellar like conditions: experimental results employing the PIRENEA setup

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Molecular photodissociation is the main limiting process for the survival of polycylic aromatic hydrocarbons (PAHs) in the interstellar medium (ISM). Upon absorption of ultraviolet (UV) photons, the excited PAH molecule can relax radiatively but can also undergo fragmentation that can lead to hydrogen loss or to the destruction of the carbon skeleton. The study of the evolution of PAH molecules under UV irradiation is then key to get insight into the properties of species that can survive in the ISM [1]. Moreover, the chemical connection between PAHs and small hydrocarbons has gained importance to account for the detection in UV-irradiated regions of species like C_3H_2, C_2H and C_4H with abundances that cannot be accounted for by gas-phase chemical models [2].

In this work, the PIRENEA (*Piège à Ions pour la Recherche et l'Etude de Nouvelles Espèces Astrochimiques*) setup [3] is used to perform photodissociation studies on a set of thirteen different PAH molecules, spanning size from two to seven aromatic rings. PIRENEA is a home-built Fourier Transform Ion Cyclotron Resonance (FT-ICR) mass spectrometer with the additional characteristics of a cold environment and low pressures to approach the physical conditions of interstellar space. Three main channels of dissociation have been determined for PAH cations, hydrogen loss, acetylene (C_2H_2) and diacetylene (C_4H_2) loss. Branching ratios of the different dissociation paths have been derived for the thirteen studied species. We will discuss the results and present some perspectives of including them in chemical models of UV-irradiated regions.

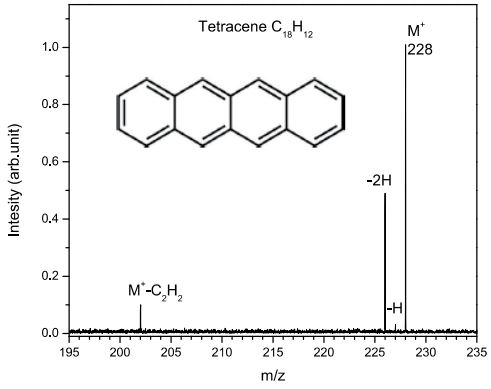

Figure 1: Photodissociation mass spectrum of tetracene employing the PIRENEA setup. Peaks associated to hydrogen and carbon losses from parent ions are identified.

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Présentation par affiche
Poster n° 23

Modelling dust in the diffuse ISM with new observational constraints from Planck HFI

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Interstellar grains are observed everywhere in our Galaxy and are associated with all the phases of the insterstellar medium (ISM), neutral and ionised, atomic and molecular. For the first time, thanks to Planck, we were able to observe variations in dust emission properties inside the diffuse ISM [1, 2], which we considered rather homogeneous until now. This finding has a great impact on our understanding of the diffuse ISM since it implies that the dust properties vary. This further influences, for instance, mass estimates in our Galaxy and also in nearby galaxies.

Observations by Planck HFI of the diffuse ISM ($N_H < 2.5*10^{20}$ H/cm^2) show variations in the dust temperature, submm opacity, and far-IR spectral index, at constant luminosity [2]. They also show that the dust near-IR to submm opacity ratio in the diffuse ISM is not compatible with standard dust models [3, 4]. However, we show that the new core-mantle dust model by [5, 6] can explain this ratio and the average properties of the diffuse-ISM dust. Additionally, allowing for small variations in mantle thickness, size distribution, carbon abundance, and metallic Fe/FeS inclusions, we show that our new dust model can explain the variations observed by Planck [7].

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Présentation par affiche
Poster n° 24

Interstellar Molecules probe the variability of the Fundamental Constants.

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The question of the time variability of the Fundamental Constants of Physics and Astronomy has been raised long ago in the frame of theories unifying Gravity with other interactions. This question came back to light after the discovery of the so called Dark Energy. Physicist realized that spectroscopic observations of remote quasars and galaxies offer a powerful way to test this variability and attempted to measure the values at high redshifts of the proton to electron mass ratio, $\mu=m_p/m_e$, and of the fine structure constant, $\alpha=e^2/\hbar c$. The first attempts were made using quasar optical lines; they implied at 4.5σ a decrease of $\Delta\alpha/\alpha$ (by $-0.5\ 10^{-5}$) over the last 10 billion years. This result, however, was disputed by subsequent reanalysis of the same data set, as well as by the analysis of new data.

Emission and Absorption lines originating inside or around quasars, more particularly optical lines, suffer from two drawbacks: the lines are broad (hundreds of km/s wide) and/or the resolution of optical spectrometers is poor. These drawbacks are largely alleviated when turning to molecular absorption lines arising in remote galaxies intercepting by chance the line of sight to a bright quasar. A few such galaxies are known. They give rise to narrow (few x 10 km/s wide) absorption features associated with the rotational transitions of interstellar molecules. The absorption lines can be detected at mm wavelengths with a very high spectral resolution.

We will review the results obtained so far on the values of the constants α and μ , as well as on the value of the Cosmic background Temperature, in two galaxies with redshifts 0.6 and 0.9.

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Présentation par affiche
Poster n° 25

New analysis methods to reveal the secrets of the Planck Galactic polarization data

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With the forthcoming release of the Planck data by the end of 2014, we are entering a new era of the polarization study. Planck will deliver the first all-sky view of the submm and mm polarized sky with a unprecedent resolution and sensitivity. While a first overview of this new open window has been published recently ([1], [2], [3], [4]) over a large fraction of the Galaxy at a resolution of one degree, we will have to face new challenges to reveal the secrets of the Planck data at full resolution over the all-sky.

We will describe how to deal with polarization measurements at low signal-to-noise ratio and what are the limitations of the usual methods to build astrophysical quantities such as the polarization fraction and angle ([5]). While these physical quantities may be strongly impacted by the properties of the noise, we will present new methods which allow to work at the full Planck resolution and in diffuse regions of the sky ([6], [7]), but also to perform statistical studies over large heterogeneous area. We will give a few applications of these methods addressing key questions related to the Galactic magnetic field and to the dust polarization properties in the ISM.

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Présentation par affiche
Poster n° 26

The relative orientation between magnetic fields and structures of interstellar matter as seen by *Planck*

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The role of the magnetic field in the formation of the filamentary structures observed in the interstellar medium (ISM) has not been elucidated yet.
For the first time *Planck* all-sky maps of linear dust polarization in emission give the possibility to study the correlation between the structure of the Galactic magnetic field and of matter, over the whole sky both in the diffuse ISM and in molecular clouds.
We will present an analysis of the Planck data that compares the projected orientation of the interstellar filamentary structures, derived from the dust opacity map, with that of the magnetic field, inferred from the dust polarization data.
We perform our analysis over two orders of magnitude in column densities, ranging from the diffuse medium up to gravitationally bound filaments.
We quantify the degree of matter structures-magnetic field alignment with analytical models that account for projection effects.
The three main results are:

(1) We estimate the ratio between the random and mean components of the magnetic field to be within 0.5 and 1.2, with a preferred value of 0.8, in agreement with an approximate equipartition between turbulent and magnetic energies in the diffuse ISM.
(2) In the diffuse ISM, we find that the interstellar structures are preferentially aligned with the local magnetic field, in agreement with what is observed in MHD simulations. This result is the most striking for structures with high polarization fraction and low column density.
(3) Alignment is less observed in molecular clouds. This result does not reflect an absence of correlation between the structures of matter and the magnetic field. Molecular clouds tend to be perpendicular to the magnetic field orientation. We will present maps that support this interpretation.

We will discuss our results in the context of theoretical studies of the formation of structures in the magnetized interstellar medium.

Présentation par affiche
Poster n° 27

CH^+ and SH^+ absorption spectroscopy with Herschel: Probing the turbulent dissipation in the diffuse ISM.

Benjamin Godard[1], Edith Falgarone[1], Guillaume Pineau des Forêts[2], Maryvonne Gerin[1], Pierre Lesaffre[1], and François Levrier[1]

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Because it is predominantly heated by the UV radiation field, the diffuse interstellar medium (ISM) has long been thought to behave like a photo-dissociation region (PDR). Yet, for the last 30 years, absorption spectroscopy has revealed a gas with a chemical richness that was unexpected from the sole predictions of PDR-type models. This problem has recently been deepened by the observations of large abundances of small hydrides using the Herschel/HIFI instrument. Since their production pathways are blocked by highly endo-energetic reactions, it has been proposed that several of these species are nothing else but a signature of another powerful energy source, such as the dissipation of magnetized turbulence [1].

Among all the molecules detected by Herschel, CH^+ and SH^+ are a unique couple [2] because the energies involved in their formation are particularly large ($\Delta E/k \sim 4640$ K and 9860 K respectively). Their presence in the cold diffuse ISM is therefore much more than a chemical riddle : it is rooted in the physics of the diffuse ISM, the intermittency of the turbulent cascade and the rate of its dissipation, and it connects with the broader issues of star formation and galaxy evolution.

The informations inferred from the absorption spectra are analysed [3] in the framework of the TDR (Turbulent Dissipation Regions) model which follows the dynamical and chemical evolutions of the gas in intermittent regions of turbulent dissipation. By comparing the predictions of the TDR model with multiwavelength observations of seven atomic and molecular species (C^+, CH^+, SH^+, H, H_2, HCO^+ and CO) we are able, for the first time, to measure five essential properties of the interstellar turbulence: (1) the dissipation rate ($\sim 10^{-24}$ erg cm^{-3} s^{-1}), (2) how it varies across the Galactic disk, (3) the size of the dissipative structures ($\sim$ 100 AU), (4) their lifetime ($\sim$ a few hundred years), and (5) the dominant dissipative process (viscous friction or ion-neutral friction).

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Présentation par affiche
Poster n° 28

The new Meudon PDR code: from galactic to extragalactic interstellar medium

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The last generation of instruments (e.g. Herschel, SOFIA, ALMA) has recently given access to the infrared and submillimeter spectra of extragalactic environments including high redshift galaxies. These observations not only reveal a chemically rich gas but also specific trends. For instance, (1) the ratio between the intensities of atomic lines and dust continuum emission shows a systematic deficit in galaxies with large star formation rate [1]; (2) several species (e.g. CO) show different excitation conditions in ULIRGs, AGNs, and starburst galaxies. Interpreting those trends is yet complex. Since the lines of sight intercepts kpc of matter, the observations necessarily include the contributions of all the phases of the interstellar medium (e.g. WIM, WNM, CNM) but also those of a variety of environments where interstellar chemistry may be driven by the radiation (PDR, XDR), the cosmic rays, or the dissipation of mechanical energy (shocks, TDRs).

Our community must now not only understand the physics and chemistry of interstellar gas in our Galaxy but also in foreign galaxies. Advanced numerical models capable of treating all scenarios are thus required. In the framework of the ANR SYMPATICO (P.I.: S. Madden), we have therefore developed a new version of the Meudon PDR code [2]. This version computes the full radiative transfer of X ray photons above 200 eV, solves their interaction with gas and dust and their subsequent impacts on the chemical and thermal structures of a cloud, and performs a new treatment of the ionization and heating of dust grains taking into account the stochastic heating of small grains and PAHs. We have already explored all these processes with a grid of several thousands models spread along five directions: the strength of the UV and X ray radiation fields, the density, the size of the cloud, and the metallicity of the gas. Each parameter spans several orders of magnitude, thus providing a full coverage of interstellar conditions.

In this talk, we will present the most recent developments of the Meudon PDR code [3] and identify for the first time the tracers of X ray dominated regions and UV dominated regions over a wide range of densities and metallicities. We will then show how this grid can be used to interpret different sets of observations as, for instance, the recent detection of ArH^+ in the Crab nebula [4]. Since the production of ArH^+ is initiated by the ionization of Argon by X ray photons or cosmic ray particles, this species could be a good tracer of X ray sources in extragalactic environments.

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Présentation par affiche
Poster n° 29

The Anatomy of a Giant Molecular Cloud

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IRAM(Grenoble and Granada), Obs. de Paris/LERMA,
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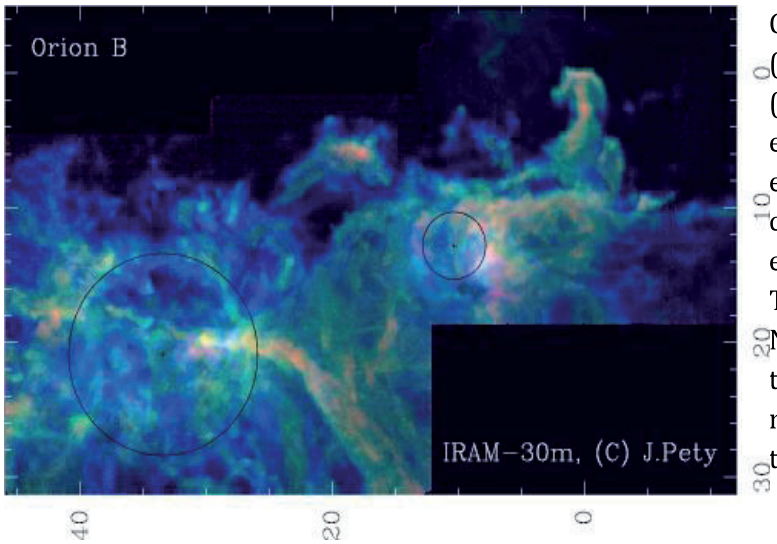
ICCM-CSIC, NRAO, Obs de Grenoble/IPAG, Cardiff University

The advent of wideband, high spectral resolution receivers turns almost any pointed observation into an unbiased spectral survey. The challenge is to use these new possibilities to classify the different kinds of environments (shocks, photo-dissociation regions, dense cores, diffuse gas, etc...) of the interstellar medium according to the molecules they contain. We aim at using signal separation techniques like those used to distinguish different kinds of geological formations from Earth satellite images.

As a test bed, we used the IRAM-30m/EMIR 3mm receiver to image 0.5 square degrees of the south-western edge of the Orion B molecular cloud around the Horsehead nebula, NGC2023, and NGC2024, with a spectral resolution of 195 kHz (0.6 km/s), a typical spatial resolution of 23'' (*i.e.*, 50 mpc or 10^4 AU at a distance of 400 pc) and a typical sensitivity of 0.1 K. We succeeded to image the isotopologues of CO as well as HCO^+, HCN, HNC, CN, CCH, C_3H_2, CS, SO, N_2H^+, SiO, CH_3OH, etc.

In this poster, we will present the data and our first results. In particular, we will show how tracers of different optical depth like the CO isotopologues will allow us to study the diffuse envelope and the dense cores, while various chemical tracers will reveal different environments (cold core, photo-dissociation regions, shocks in potential outflows, etc).



Composite image of the ^{12}CO (blue), ^{13}CO (green), and $C^{18}O$ (red) integrated line profile emission of the south-western edge of the Orion B molecular cloud. The Horsehead nebula emerges in the top right part. The emblematic NGC 2024 and NGC 2023 objects are marked as the large and small circles respectively (IRAM-30m telescope at Pico Veleta, Spain).

Présentation par affiche
Poster n° 30

Does the halo of our Galaxy possess an X-shape magnetic field?

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The magnetic field is an important component of the interstellar medium. It plays a major role in a variety of physical processes (hydrostatic balance, star formation, cosmic-ray acceleration and propagation...), but its properties remain poorly understood. Radio observations of nearby galaxies similar to the Milky Way reveal common features such as field lines with an "X-shape" structure in their halos. This finding quite naturally raises the question of whether the halo of our own Galaxy possesses an X-shape magnetic field. In this talk, we will present a study in which we use analytical models of divergence-free, X-shape magnetic fields to simulate all-sky maps of the Galactic Faraday depth. The few free parameters of the models are adjusted to provide the best possible fit to the observational data. The observational all-sky map of Faraday depth that we use as a reference contains a lot of detailed information (on small-scale fluctuations in the magneto-ionic ISM) that is irrelevant to the large-scale magnetic field structure. Therefore, we bin the Faraday depth data and average them within the different bins. We also implement a statistical approach to estimate the uncertainty in the average Faraday depth values arising from the turbulent magnetic field. This uncertainty, combined with the measurements errors, enable us to define the appropriate χ^2 criterion to test our models.

Présentation par affiche
Poster n° 31

The Herschel/HIFI insight on the CH+(1-0) puzzle in the diffuse medium.

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We have extended the CH^+(1-0)absorption measurements performed within the Herschel/HIFI PRISMAS Key Program to the most tenuous phases of the interstellar medium, taking advantage the high opacity of this transition in the diffuse medium. We targeted the nuclei of three galaxies, M82, NGC 4945 and Circinus and star forming regions in the outer Galaxy. The former observations probe diffuse gas within the target galaxies but also in our Galaxy, over a broad range of distances from the plane, down to gas column densities as low as a few 10^{20} cm^{-2}.

CH+ absorption has been detected in all these environments. The CH^+(1-0) absorption lines in the two former galaxies are close to saturation and cover the whole velocity range of the hydrogen 21cm line emission. The negative velocities of the CH^+(1-0)absorption lines against Circinus and NGC 4945 reveal the presence of CH^+ at 200 pc (or more) above the plane, i.e. in the thick molecular disk . The H_2 fraction is inferred from the CH absorption lines.

These results confirm the presence of molecules in extreme, low column density environments with low molecular hydrogen fraction, therefore poorly shielded from the UV photons. They further promote new chemistry models in which some of the very first steps of chemistry in the diffuse medium are triggered by local and intense releases of turbulent energy (see the abstract by Godard et al.).

We will discuss the implications of these results for the transfer of energy and the dynamics of the extended low density molecular medium, in our Galaxy and external galaxies.

Présentation par affiche
Poster n° 32

Interstellar silicate grain analogs: spectroscopic study at different temperatures from MIR to submm

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Big grains of size ~0.1μm dominate the continuum emission of the ISM (Interstellar Medium) in the spectral domain from 100 μm to 1000 μm. They are mostly composed of amorphous silicate and carbonaceous matter. The dust grains give us important information about their physical-chemical environment, they trace the ISM structure, catalyze the molecule formation… However, our understanding of interstellar grains is not perfect. In particular, the widely used modified blackbody model describes the dust emission as $I_\nu = \kappa \nu^\beta B_\nu(T)$ with the dust emissivity spectral index being independent of temperature with a single value~2, while the PRONAOS observation and the early results of Planck and Herschel suggest β-T are anti-correlated.

Our aim is to study the optical properties of analogs of these interstellar grains (dust grains synthesized in laboratory with different methods: sol-gel, glass, smoke…) with laboratory spectroscopic measurements, so as to contribute to the interpretation of observational data.

We carried out our measurements on the experimental setup ESPOIRS located at IRAP. We measured the spectra of the glassy amorphous composite silicate grains of composition (1-x)MgOxSiO$_2$ (with x = 0.35, 0.36, 0.40, 0.41, 0.50) of submicronic and micronic size and in the spectral range from medium infrared to far infrared (8-1000μm). We obtained their optical properties at different temperatures (10-300K), compared the spectra of analogs synthesized by glass and by sol-gel methods and investigated the influence of grain size distribution, temperature and chemical composition on the mass absorption coefficient. These experimental optical constants at low temperature of silicate dust analogues will be useful for the astronomers to understand correctly the physical-chemical properties of interstellar dust, to improve the dust models for a better interpretation of observation.

Présentation par affiche
Poster n° 33

The kinematics and physical properties of a single, diffuse cloud observed from within, and how the cloud responds to the surrounding environment

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UV absorption lines appearing in the spectra of nearby stars indicate that the heliosphere is surrounded by a single, coherent medium with an internal density that varies from 0.03 to 0.1 cm^{-3} and an outer boundary that is somewhat irregular and located about 9 pc away from us in all directions. Most of the gas is moving at a velocity and direction that is consistent with other determinations of the very local flow approaching the heliosphere. This cloud that surrounds us affords a unique opportunity to study a small volume of the diffuse medium without the confusion arising from other clouds in the sight line.

Small kinematical deviations away from the mean velocity vector indicate that the cloud does not behave like a rigid body: it appears to be undergoing a differential deceleration (i.e., compression) in the direction of motion and an expansion in perpendicular directions, much like a squashed balloon. The metal abundances decrease steadily from the rear to the head of the cloud, and this phenomenon does not appear to be related to ionization effects.

Within the volume occupied by this cloud, there are additional, secondary velocity components that are not part of the main flow. Half of them exhibit evidence for internal motions that progress toward the interior parts of the cloud at a velocity of 7 km/s. These components cover about half of the sky. They are consistent with flows behind a shock wave that may have been driven by an enhancement of thermal or magnetic pressures in a much lower density medium that surrounds the cloud.

Présentation par affiche
Poster n° 34

Exploring Water Dimer Formation

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Water is ubiquitous within the universe (Sun, interstellar clouds, circumstellar envelopes, protostars, planets …)as observed by Herschel[1] and previous space telescopes. Water dimers are likely to be present in comets, where they could affect the variety of hydrated ions[2]. From a fundamental point of view, the water dimer is a benchmark for understanding H-bonding mechanisms in molecules and clusters. Furthermore, water dimer formation is the first step in the homogeneous nucleation process of water vapour. Finally, water dimers may be responsible for the apparent deficit in the atmospheric absorption of solar radiation.

In the laboratory, we have explored the dimerization kinetics by measuring the associative coefficient of two water molecules at low temperatures. This study has been conducted with the help of a dedicated CRESU (Cinétique de Réaction en EcoulementSupersoniqueUniforme) chamber combined with a time of flight mass spectrometer. Supersonic uniform flows are well adapted to explore low temperature reaction kinetics. The kinetics of water dimer formation has been investigated over the 23 to 70 K temperature range. The combination of the experimental results with theoretical calculations will lead to the determination of the equilibrium constant of the reaction and of the dissociation energy of the water dimer as well as the pressure dependence of the rate coefficient.

Future work includes the coupling of the CRESU with infrared CW-CRDS (Continus Wave-Cavity Ring Down Spectroscopy) for absolute detection of products. This should open the way to the investigation of other molecules of astrophysical interest such as ethane, propane and acetylene which are for instance suspected to play an important role in the formation of aerosols in Titan's atmosphere.

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Présentation par affiche
Poster n° 35

Modeling ionized PAH clusters: structures, thermodynamics and spectroscopy

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Polycyclic Aromatic Hydrocarbons (PAHs) are the carriers of the aromatic IR emission bands that are observed between 3 and ~15 μm in the interstellar medium. Observations suggest that PAHs are produced from the evaporation of very small grains (possibly PAH clusters) under the irradiation of UV photons [1].

We have investigated the properties of ionized PAH clusters. Density Functional based Tight Binding (DFTB), which is an approximated method of Density Functional Theory (DFT), is used to reduce computational time on these large systems [2]. We have adapted the DFT-CI approach [3] to the DFTB scheme [4,5] together with long-range dispersion and inter-molecular polarization corrections to treat ionized PAH clusters up to 10 units. A global exploration by Parallel Tempering Monte Carlo [6] of the potential energy surface permits the identification of characteristic patterns for both structure and charge distribution, which is validated by recent experimental results obtained at SOLEIL on the ionization potentials.

We have extended the DFTB-CI combination to localized configurations involving holes in several orbitals below the Fermi level to determine charge resonance excited states. We will show results on benzene, pyrene or coronene cationic clusters and provide a first comparison with photoelectron spectra obtained at SOLEIL on the last two species.

Acknowledgments: ANR GASPARIM (ANR-10-BLAN-0501), CALMIP-CICT (computational facility), GDR EMIE (GDR 3533).

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Présentation par affiche
Poster n° 36

Breakdown curves of carbon-based molecules for astrochemistry

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Carbon-based molecules are ubiquitous in astrophysical environments. A collaboration between experimentalists and theoreticians aims at providing to the astrochemistry community branching ratios (BR) for important physical (photo-dissociation, dissociative recombination) and chemical (neutral-neutral, ion-neutral, ion-pair) processes involving carbon and hydrocarbon species.

The experimental group in Orsay (France) has developed a dedicated set-up (AGAT) for fragmentation recording of molecules and clusters of known charge and internal energy. Recently they showed how these data could be used to provide, within a statistical fragmentation context, BR for numerous physical and chemical processes of astrophysical interest. The method relies on the construction of Breakdown curves (BDC, which are energy dependent BR) constrained by the experimental measurements. With this method, BRs for reactions forming $C_n^{(0,+)}$ species (n=3-10), $C_nH^{(0,+)}$ species (n=1-4) and $C_3H_2^{(0,+)}$ species were extracted [1].

In the future, BDC for all $C_nH_m^{q+}$ species (n≤5, m≤4 q≤2) will be theoretically constructed by the Madrid group and benchmarked with new measurements of the Orsay group. BR of processes involving these species in the ISM will be then derived. These BR will be included in the international astrochemical database KIDA (http://kida.obs.u-bordeaux1.fr). Also the impact of extracted BR in some astrophysical environments (dark clouds and photo-dissociation regions) will be studied.

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Présentation par affiche
Poster n° 37

Experimental formation of H_2 via reactions on PAHs

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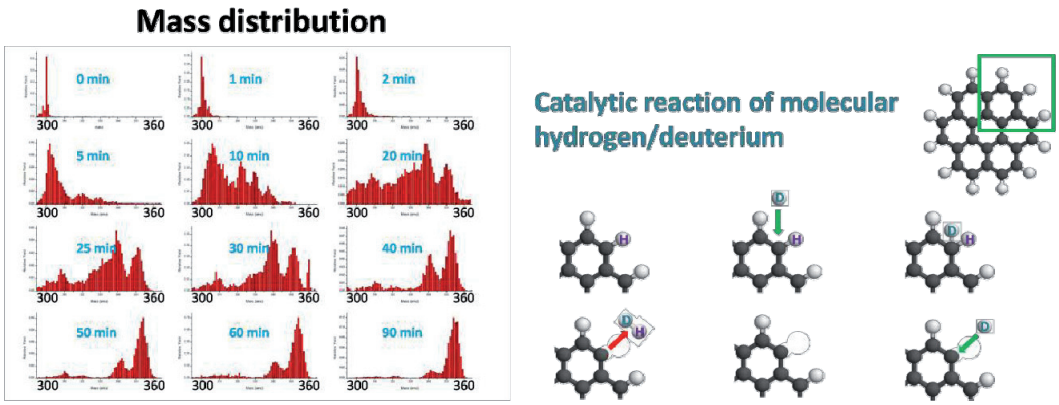
H_2 is the most abundant molecule in the interstellar medium, but there is no efficient gas phase formation route, as density is too low. We expect larger molecules, like PAHs, to act as catalysts for the molecular hydrogen formation.

DFT calculations **[1]** indicate a possible formation process of H_2 in such condition, we experimentally investigated this by deuterating coronene molecules with an atomic source, varying exposure time and atoms temperature, and probed results of the reactions using temperature programmed desorption and mass spectrometry.

Results confirm that full deuteration of coronene occurs with high deuterium doses, and there are some preferred configurations in the deuteration pattern, depending of the dose, and hydrogen atoms are replaced, indicating the formation of hydrogen molecules.



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Présentation par affiche
Poster n° 38

De l'invariabilité des constantes universelles
Le cas de la constante hyperfine

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En 1999, Webb et ses collaborateurs, suite à l'analyse de lumière provenant de quasars lointains, affirmèrent avoir « observé » une variation de la constante de structure fine . Aucune étude ultérieure ne confirma ce résultat.

Avec les méthodes de la chimie quantique, nous avons simulé des variations de cette constante α à la fois dans le cadre d'un modèle non-relativiste et d'un modèle relativiste, et avons évalué quantitativement la réponse spectrale à ces variations. Nous avons montré que dans le cadre du modèle non-relativiste le décalage spectral induit par ces variations n'était en fait pas décelable observationnellement et se voyait absorbé dans ce qui est attribué au redshift habituel, mais que dans le cadre du modèle relativiste il apparaissait un déplacement spécifique éventuellement observable.

Nous avons été amenés à définir deux types de réponses à une éventuelle variation de α: l'une qualifiée de théorique et l'autre d'observationnelle. La première approche prévoit la réponse à la variation de α à la fois dans la partie non-relativiste et dans la partie relativiste de l'énergie de transition et fournit ainsi une indication sur ce que nous avons appelé le décalage théorique global. La seconde approche ne tient compte que du décalage spécifique induit par la variation de α dans le cadre du modèle relativiste et donne une indication sur ce que nous avons appelé le shift observationnel.

Nous présentons un protocole permettant de déterminer les décalages induits par une variation de la constante de structure fine à partir du spectre électronique calculé à variation nulle, aussi bien pour des molécules que des atomes.

Dans tous les cas étudiés, les résultats obtenus selon ce protocole montrent qu'une variation de α de l'ordre de celle que J. Webb affirme avoir détectée, induirait des déplacements de raies minimes qui ne seraient pas décelables par les appareils d'observation actuels, leur résolution étant trop faible.

Présentation par affiche
Poster n° 39

A method to measure CO and N_2 depletion profiles inside prestellar cores

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In the dense and cold prestellar cores, many species freeze out onto grains to form ices. The most conspicuous case is that of CO itself, the standard tracer of molecular gas. Only upper limits of this depletion amplitude can be estimated because the CO emission from the external undepleted layers mask the emission of CO left inside the depleted region. The finite signal-to-noise ratio of the observations is another limitation. However, depletion and even more desorption mechanisms are not well-known and need observational constraints, i.e., depletion profiles.

We recently developed a method for retrieving the CO and N_2 abundance profiles inside prestellar cores, which is mostly free of initial conditions : it is based on the observations of DCO^+ which is a daughter molecule of CO, and which appears inside depleted prestellar cores. The main deuteration partners are the H_3^+ isotopologues. By determining the abundance of these isotopologues via N_2D^+, N_2H^+, and ortho-H_2D^+ observations and a chemical model, we can uniquely constrain the CO abundance, the only free parameter left, to fit the observed DCO^+ abundance. The N_2 abundance is also determined in the same manner once CO is known.

To illustrate the method, we applied it to the main L183 prestellar core (Fig .1) and find that the CO abundance profile varies from $\geq 2.4 \times 10^{-5}$ at the core edge to $\leq 6.6 \times 10^{-8}$ at the center. This represents a relative decrease in abundance by ≥360, and by ≥2000 compared to the standard undepleted CO abundance ($1–2 \times 10^{-4}$). Comparatively, N_2 abundance decreases much less, from $\leq 3.7 \times 10^{-7}$ down to $\sim 2.9 \times 10^{-8}$, in contrast to the similar binding properties of the two species. Because the N_2 abundance is lower than its steady state value at the edge, while CO is close to its own, a possible explanation is that N_2 is still in its production phase in competition with depletion.

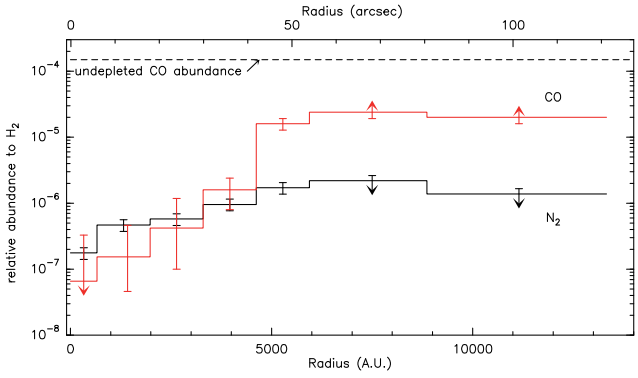

Figure 1 CO & N_2 profiles towards the L183 main prestellar core

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Présentation par affiche
Poster n° 40

Hydrogen atom abstraction reactions in the interstellar medium

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This work reports the results of the hydrogen atom abstraction reaction $CH_4 + N(^4S) \rightarrow CH_3 + NH$ in the ground state, at very low temperatures (3K-20K), with no additional energy, monitored via an FTIR spectrometer. A beam of ground state N atoms has been generated with a microwave discharge plasma in nitrogen and further co-condensed with methane. Under cryogenic temperatures and with a classical barrier height theatrically predicted at 33 kcal.mol^{-1}, the reaction of CH_4 with $N(^4S)$ should not occur spontaneously and require an initiating energy. However, the detection of some byproducts such as the free CH_3 radicals in our solid samples, left in the dark for hours at 10 K, is an evidence of a hydrogen abstraction reaction from a C–H bond. Our results show the efficiency of CH_3 radical formation stemming from non-energetic N-atoms and CH_4 molecules, and such reactions, that may occur on the surface of dust grain ices in dense molecular clouds, cloud be the first key step towards complex organic molecules production in the interstellar medium.

Présentation par affiche
Poster n° 41

Solid-gas equilibrium investigated by means of spectroscopic measurements at relevant temperatures for cold interstellar objects

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The sublimation and condensation of ices play a very important role in the formation of planetary systems, in the evolution of some solar system bodies as well as in the equilibrium and matter exchanges between surface and atmosphere of most planets and satellites. Pure or nearly pure ices of volatile species can exist at equilibrium on several objects of the outer solar system. The precise knowledge of vapour pressure of molecular solids at all relevant temperatures is mandatory.

We propose in this study a sensitive method to derive the temperature and pressure of a molecular gas enclosed in equilibrium with its solid in low-temperature cells by comparing experimental and modeled gas phase IR absorption spectra. We used two different set-ups: one with a home-made high resolution spectrometer (<0.001 cm^{-1}, path length = 692 cm) [1], which is used as a reference and one with a commercial low resolution spectrometer (≈0.12 cm^{-1}, path length=1.8 cm). We applied our methodology to determine the Clapeyron solid-gas equilibrium curve for methane in the range 40-80 K, using four ro-vibrational transitions in each of the ν_3, $\nu_3+\nu_4$, $\nu_1+\nu_4$, $\nu_2+\nu_3$ vibrational bands.

We found the same curve as in the literature in the range 50-80 K, obtained with both low and high resolution set-ups [2]. In addition, we extended these data by new measurements, obtained with the high resolution set up, in the range 40-45 K, corresponding to pressures in the range $5\text{-}20\times10^{-6}$ Torr. This demonstrates the ability of this technique for fine quantification of low pressure gas. Using this method with a high resolution set-up and a higher number of transitions will allow for a new and/or extended Clapeyron curve determination for temperature range of astrophysical interest. Inversely, for previously explored temperature range, the deviation from the Clapeyron curve could allow for a more precise determination of the spectral line intensities.

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Présentation par affiche
Poster n° 42

Hyperfine excitation of C_2H and C_2D by para-H_2.

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Ethynyl radical (C_2H) is one of the most abundant molecules in the interstellar medium (ISM) [1,2]. C_2H and it associated isotopologue C_2D are frequently used to study the physical conditions of cold molecular clouds [3]. In particular, they can be used to trace D/H ratio in these media [4]. Accurate determination of their abundance in the ISM requires to model the collisional excitation of these species by H_2.

In this poster, we report theoretical calculations of cross sections and rate coefficients for the collisional excitation of C_2H and C_2D by para-H_2(j=0). The two molecules were treated as rigid rotors. A new accurate potential energy surface has been computed from highly correlated *ab initio* calculations. Close-coupling calculations of the collisional cross sections between the first 17 fine-structure levels of C_2H and C_2D were performed. Corresponding rate coefficients up to 80 K were then computed. The results show significant differences between the two species. In particular, C_2D data seems to be lower in magnitude than the C_2H ones.

Using nuclear spin free collisional S-matrices and angular momenta recoupling techniques, collisional cross sections and rate coefficients between hyperfine levels of C_2H and C_2D were obtained. The propensity rules between hyperfine levels were investigated. It is found that $\Delta j=\Delta F$ transitions are the strongest ones.

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Présentation par affiche
Poster n° 43

Collisional excitation of CO by H_2, D_2 and He : On the validity of theoretical models for interpreting astrophysical observations.

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CO molecules are of particular interest due to their crucial role in astrochemistry. Modeling of CO spectra from interstellar clouds requires the calculation of rate coefficients for (de-)excitation by collisions with the most abundant species, H_2 and He. This is usually achieved from potential energy surfaces (PES). However, theoretical calculations predict that rotational energy transfer to small molecules, such as CO, by collisions with H_2 or He is dominated by resonance phenomena, which can only be revealed at very low energies[1]. Experiments conducted with a crossed, molecular beam apparatus with variable crossing angle allowed the integral cross sections (ICS) to be determined as a function of the relative translational energy down to a few wavenumbers, *i.e.* below the threshold of the {j = 0 - 1} CO transition at 3.85 cm^{-1} (5.5 K). The experimental results, which exhibit behaviours characteristic of quantum resonances, are compared to QM scattering calculations. Agreement with theory is shown to strongly depend on the characteristics of the potential energy surface (PES) used to perform the QM treatment. For the CO(j=0) + p-H_2 → CO(j=1) + H_2, ICS were calculated with the new PES developed by P. Jankowski, A. R. W. McKellar and K. Szalewicz[2] and will be compared to our experimental data[3]. Our recent studies of inelastic scattering of CO with n-H_2, o-D_2, n-D_2 and He will also be presented.

This work has been supported by the French National Research Agency (ANR-**HYDRIDES,** ANR-12-BS05-0011-01 contract), the Conseil Régional d'Aquitaine (contract 2007.122) and the PHC Van Gogh ("Cold Collisions", n°28484TH).

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Présentation par affiche
Poster n° 44

The collisional excitation of ammonia and its deuterated isotopologues revisited.

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Ammonia is an important interstellar molecule, which has been observed in many different astrophysical environments. Apart from its important role in the nitrogen chemistry, this molecule is a good probe of the physical structure of the objects observed, since its emission is particularly sensitive to the gas temperature [1, 2].

In studies analysing ammonia emission line intensities, the knowledge of state to state excitation rates in collision with H_2, is a pre-requisite to obtain reliable estimate of the object physical structure (i.e. gas temperature, H_2 densities, ammonia abundance, ...). At low temperature, para-H_2 is the most important collider. However, as temperature increases, the ortho-H_2 molecules tend to dominate the collisional excitation, because of the increasing abundance and collisional efficiency of the ortho-H_2 species .

In the current study, we report the calculation of new collisional rate coefficients for NH_3 and its deuterated isotopologues NH_2D and ND_2H. For ammonia, specific calculations were performed for both ortho and para-H_2, since both colliders can play an important role depending on the temperature of the object. However, since the observations of deuterated isotopologues mainly focus on cold objects [3], we restricted our calculations to para-H_2 molecules for these species. In the particular case of NH_2D we estimate the ortho H_2 rate coefficient from the para H_2 (j=2) rate coefficients. The current calculations improve the earlier estimates of the NH_3 isotopologues collisional rate coefficients (either estimated with He or with para-H_2 (j=0) [2, 4, 5, 6]. Given the differences observed with earlier calculations, especially in the case of the deuterated isotopologues, we expect that these new rate coefficients will improve the analysis of the ammonia emission in astrophysical objects.

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Présentation par affiche
Poster n° 45

Weak maser action in interstellar methyl formate

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A non-LTE radiative transfer treatment of *cis*-methyl formate ($HCOOCH_3$) rotational lines was presented recently using a set of theoretical collisional rate coefficients [1]. These coefficients were computed in the temperature range 5-30 K by combining coupled-channel scattering calculations with a high accuracy potential energy surface for $HCOOCH_3$ - He [2]. The results were compared to observations toward the Sagittarius B2(N) molecular cloud using the publicly available PRIMOS survey from the Green Bank Telescope [3]. A total of 49 low-lying transitions of methyl formate, with upper levels below 25 K, were identified. We will show that these lines probe a presumably cold (~30 K), moderately dense (~ 10^4 cm^{-3}) and extended region surrounding Sgr B2(N). The derived column density of ~ $4 .10^{14}$ cm^{-2} is only a factor of ~ 10 larger than the column density of the *trans* conformer in the same source [4]. Provided that the two conformers have the same spatial distribution, this result suggests that strongly non-equilibrium processes must be involved in their synthesis. Finally, we will show that all detected emission lines with a frequency below 30 GHz are (collisionally pumped) weak masers amplifying the continuum of Sgr B2(N). This work thus provides the first theoretical support for maser action in the rotational spectra of complex organic molecules at centimetre wavelengths.

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Présentation par affiche
Poster n° 46

A detailed radiative transfer study of nitrogen bearing molecules.

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Rotational spectra of nitrogen bearing molecules are spectroscopically complex, because of the hyperfine structure induced by the spin of the nitrogen nucleus. In practice, reproducing the relative intensities of the hyperfine of a rotational transition puts strong constraints on their relative opacities, and hence gives useful informations on the physical (gas temperature, density) and chemical (molecular abundance) structure of the source [1].

In the current study, we present the analysis of Herschel observations of NH, NH_3 and their deuterated isotopologues in the L1544 [2] and I16293E [3] prestellar cores. These analysis are based on the newly available collisional rate coefficients for the NH_2D / H_2 collisional system [4]. Most importantly, these studies rely on a detailed radiative transfer treatment, which takes into account the line overlap between the hyperfine transitions [5]. While introducing this effect has only marginal consequences on the analysis of the NH_3 isotopologues, we conclude that the ND line is on the contrary quite sensitive to it [3]. Indeed, variations in the line intensities of a factor ∼2 are obtained between the models that consider or neglect line overlap. Finally, in the view of the current modeling, we briefly discuss the nitrogen and deuteration fractionation chemistry at work in these objects, as well as the kinematics of the cores, which is inferred from the line profile analysis.

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Présentation par affiche
Poster n° 47

Modeling the magnetic field structure of interstellar filaments using Planck dust polarization observations

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Herschel dust continuum images have revealed the ubiquity of filaments in the interstellar medium and their fundamental role in the star formation process. Much progress has been made in the past few years on the formation and evolution of the filamentary structures out of diffuse interstellar medium. Now, with the Planck satellite, we have access to maps of dust polarized emission associated with these filament, which provide crucial information on the structure of the magnetic field of the filaments and their host molecular clouds.

I will show Planck observations at 353 GHz towards nearby interstellar filaments. I will present the modeling of the observed polarized emission of the filaments and their surrounding clouds assuming constant intrinsic dust polarization. The observed dust polarized emission of the filaments is successfully modeled with a uniform magnetic field intrinsic to the filament combined with a different field orientation for the local cloud. Hence, the observed polarized emission may be accounted for by a simple description of the three dimensional (3D) geometry of the magnetic field, with the same polarization efficiency of the dust grains in the cloud and in the filament.

The observed and modeled polarization fractions are smaller in the filaments compared to that of their surrounding environment. We show that this drop in the polarization fraction may result from the 3D structure of the magnetic field.

The magnetic field in the filaments is found to be different than that of the surrounding clouds. This result suggests that the magnetic field of the molecular cloud may be influenced by the formation of the filamentary structures: The field structure evolves as the filament forms. We suggest that the difference between the present field geometry in the filament and that of the parent cloud may arise 1) from interstellar shears, which drag the matter and the field lines of the cloud differently than the field in the denser filament, 2) from gas accretion due to magnetic flux conservation.

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Présentation par affiche
Poster n° 48

Excitation and chemistry of interstellar hydrides: the ANR project hYdRiDeS

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Hydrides play a central role in astrochemistry as significant reservoirs of heavy elements. Excitation studies of interstellar hydrides deserve a particular attention because the reactive processes with the most abundant colliders (electrons, H and H_2) can compete with or even dominate the energy transfer processes. The objective of the cross-disciplinary ANR project hYdRiDeS (2013-2016) is to address this challenging problem both theoretically and experimentally [1]. In addition to the production of fundamental molecular data, the analysis of available astronomical spectra, especially from the Herschel space telescope, is our second objective. Such studies have been so far hampered by the lack of accurate collisional cross sections and rate coefficients for the relevant species. We will present the most recent results of the project, with a special emphasis on comparisons between theoretical and experimental state-specific cross sections.

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Présentation par affiche
Poster n° 49

Chemistry in Protoplanetary Disks

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Studying the chemical structure and evolution of protoplanetary disks is essential for our understanding of planet formation. Fundamental disk properties, such as disk temperature and mass or molecular content and distribution, are still poorly constrained. As the main constituent, H_2, cannot be observed, we rely on indirect tracers, principally simple molecules to derive the disk characteristics.

We report here a sensitive search for several molecules HCN, HNC, HC_3N, N_2H^+, CS, $C^{34}S$ and CCS in four protoplanetary disks sampling different age and physical conditions: the T Tauri DM Tau, GO Tau and LkCa 15 and the Herbig Ae MWC 480. The survey was made using the broad band correlator (FTS) of the IRAM 30-m radiotelescope. Together with our lines of interest we observed with the same correlator setup ^{13}CO, $C^{18}O$, HCO^+, H_2CO and DCO^+.

We compare the observational results with predictions coming from the chemical model NAUTILUS (Hersant et al. 2009; Semenov et al. 2010) in which both gas-phase and grain-surface reactions occur. The chemical network used for this work was recently updated based on Loison et al. (2014) and Wakelam et al. (2013). We find that better agreement with the observations is obtained with the updated network and a C/O ratio of 0.55 for an initial cloud H density of 2×10^4 cm^{-3} and age of 5×10^6 yr.

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Présentation par affiche
Poster n° 50

Physical properties of an externally illuminated protoplanetary disk in the Carina Nebula: a case study with Herschel.

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Most low and intermediate mass stars are born within transient OB associations [1], and very likely the Solar System too. In such environments, protoplanetary disks around young stars are ionized and photoevaporated by ultraviolet photons (UV) arising from nearby massive stars, forming objects known as "*proplyds*" [2]. The expected short lifetime of such disks may be an issue for the formation of gas giant planets that could take place in them. Here, we present an analysis of such an object based on infrared (IR) observations obtained with the Herschel space telescope as part of an open time program dedicated to *proplyds*. The study was focused on a *proplyd* located in the Carina nebula, for which several gas lines (*i.e.* [CII], [OI], and some high-J CO lines) have been detected with the instruments PACS and HIFI. The spectral energy distribution of dust emission was also extracted from PACS data. We modeled the gas line emission using the Meudon photodissociation region (PDR) code [3] while the dust emission was modeled with simple modified black-bodies as a first crude approximation. Both the gas and dust emission is well reproduced with two components, a model comprised of a dense (10^7 cm^{-3}) and massive molecular disk, surrounded by a diffuse (about 10^4 cm^{-3}) atomic envelope. We will discuss the implications of our results on the understanding of the physical evolution of proplyds in the context of planet formation.

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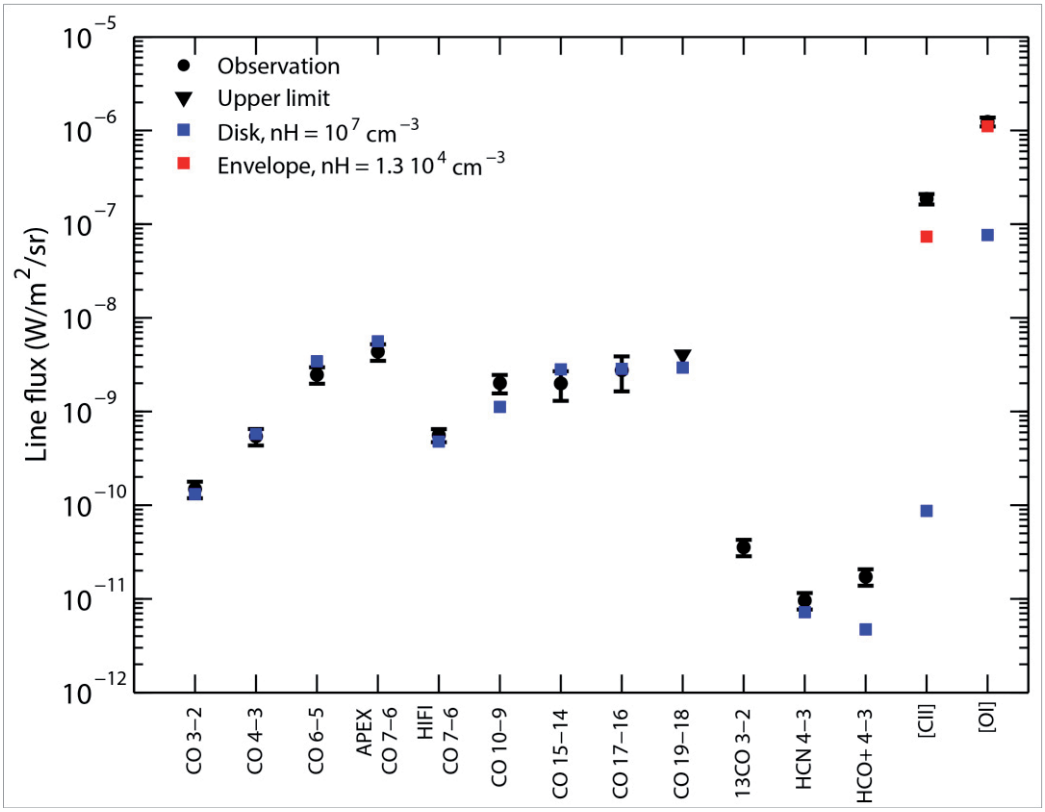

Figure 1. Observed (black) gas emission for the studied *proplyd* and modeled values (blue and red) obtained by the Meudon PDR code [3]. Some data come from previous observations obtained with the Atacama Pathfinder Experiment 12-m telescope [4].

Présentation par affiche
Poster n° 51

Interstellar chemistry of nitrogen hydrides revisited with the Herschel Space Observatory

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Nitrogen, amongst the most abundant metals in the interstellar medium, has a peculiar chemistry that differs from those of carbon and oxygen. Observations of several nitrogen-bearing species in the interstellar medium suggest abundances in sharp disagreement with current chemical models. Although some of these observations show that some gas-grain processes are at work, gas-phase chemistry needs first to be revisited. Strong constraints are provided by *Herschel* observations of nitrogen hydrides in cold gas [1]. The aim of my PhD thesis work was to comprehensively analyse the interstellar chemistry of nitrogen, focussing on the gas-phase formation of the smallest polyatomic species and, in particular, on nitrogen hydrides. We present a new chemical network [2] in which the kinetic rates of critical reactions have been updated based on recent experimental and theoretical studies, including nuclear spin branching ratios [3]. Our network thus treats the different spin symmetries of the nitrogen hydrides self-consistently, together with the ortho and para forms of molecular hydrogen [4]. This new network is used to model the time evolution of the chemical abundances in cold and dense gas conditions (n=10^4 cm^{-3}, T=10 K). The steady-state results are analysed, with special emphasis on the influence of the overall amounts of carbon, oxygen, and sulphur. Our calculations will be compared with *Herschel*/HIFI observations of NH, NH_2, and NH_3 towards a sample of low-mass protostars.

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Présentation par affiche
Poster n° 52

Excitation and recombination of molecular cations of astrophysical interest with electrons: application to H_2^+, CH^+ and N_2^+

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In the chemical modeling of the kinetics of the early Universe, interstellar media and planetary atmospheres, rate coefficients for elementary reactions are badly needed [1-4]. Meanwhile, in diffuse environments, electrons are expected to be the dominant exciting species for molecular ions, as the cross sections for electron impact excitation are several orders of magnitude larger than those corresponding for excitation by neutral atomic or molecular species. Cation excitation is competed by dissociative recombination, a major process for the charged particle kinetics [5].

Using the Multichannel Quantum Defect Theory (MQDT) [6] and the Adiabatic-Nuclei Rotation (ANR) approximation [7], cross sections and rate coefficients have been obtained for rotational transitions induced in H_2^+ and HD^+ molecular ions [8]. New data on vibrational transitions in CH^+ and N_2^+ [9] ions have been produced, following a careful study of the role of the core-excited Rydberg states. For all these systems, dissociative recombination data have also been obtained, and comparison with measurements in CRYRING and TSR heavy-ion-storage-rings resulted in a very good agreement.

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Présentation par affiche
Poster n° 53

Photofragmentation of H_2 of astrophysical interest: mechanisms and cross sections

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The diatomic molecular hydrogen is a dominant molecule in the interstellar molecular clouds and a basic building block in the chemistry of the Early Universe. The modeling of these environments relies on accurate cross sections for the various relevant processes. Among them, the photoionization and the photodissociation play a major role in the kinetics and in the energy exchanges involving H_2 [1, 2].

We report theoretical photoionization cross sections for vibrationally relaxed ($v'' = 0$) or excited ($v'' > 0$) levels of its electronic ground state [3]. Our multichannel quantum defect theory (MQDT) calculations take account of the full manifold of Rydberg states and their interactions with the electronic continuum. We show that the photoionization cross section is dominated by resonance effects, in the sense that autoionization resonances are responsible for the major part of its value. Indeed, inclusion of these resonances leads to an increase by an order of magnitude of the photoionization rate with respect to the contribution of the flat continuum, a fact that might have significant consequences in the framework of current astrophysical models.

The present work deals on one hand with photoionization from vibrationally excited levels, more specifically with the Q transitions ($N' = N''$) which account for roughly one third of the total photoabsorption cross section. On the other hand, we extend the calculations to P- and R-transitions ($\Delta N = -1$ and 1 respectively), which requires inclusion of simultaneous ionization (I) and dissociation (D) processes, both of which are far stronger than in the case of the Q transitions. The interconversion of electronic and nuclear energy is mediated by bound states embedded in the "I+D" continua. We have developed [4] a reactive scattering version of MQDT, which treats discrete series of states and multiple fragmentation continua in a unified fashion. We shall show results on the predissociated levels corresponding to $3p\pi D\ ^1\Pi_u$ $v' > 3$, $N' = 1,2$ R-transitions. Our calculated resonance profiles are in excellent agreement with those obtained in recent experiments on the SOLEIL, Saclay and BESSY II Berlin synchrotrons [5, 6].

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Présentation par affiche
Poster n° 54

Diffusion and chemistry of O atoms at very low temperatures on surfaces of astrophysical interest

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Recent experimental works carried out by our group at LERMA Cergy confirmed that not only the mobility and reactivity of H atoms contribute to the complexity of surface chemistry, but also oxygen atoms can diffuse fast at the low temperatures of interstellar dust grains [1-4].

In this talk, I will present a summary of the laboratory works about O-atom diffusion and reactivity on a variety of astrophysically relevant surfaces (water ice of three different morphologies, silicate, and graphite) in the 6.5–25 K temperature range. We compared the experimental values of the diffusion coefficients and found that the rates of diffusion on each surface, based on modelling results, were considerably higher than those expected for heavy atoms such as oxygen. The implications of efficient O-atom diffusion over astrophysically relevant time-scales will also be discussed. Our findings show that O atoms can scan any available reaction partners (e.g., either another H atom, if available, or a surface radical like O, OH, CO) at a faster rate than that of accretion. In particular, in very dense interstellar clouds, the O/H ratio is such that O becomes one of the dominant reactive partners together with H. This has an impact on the chemistry occurring at the surface of dust grains as either the formation of some species may be enhanced, or at least the relative abundances of the final products will be affected. An important example of how O-atom mobility can modulate the abundances of key species of ices in the ISM is the case of the H2O/CO2 ratio via the CO+O and H2CO+O pathways [5-6].

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Présentation par affiche
Poster n° 55

Low temperature water cluster formation: results and prospect.

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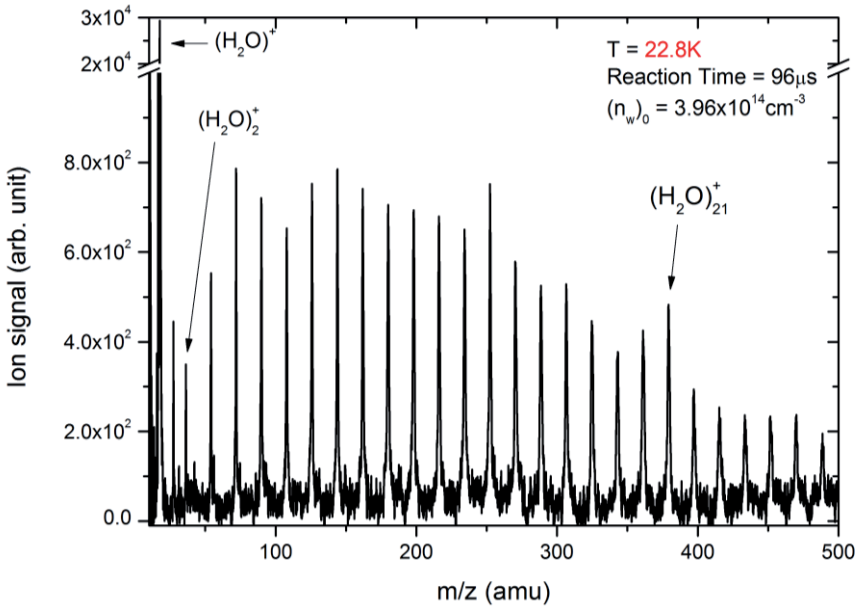
The universe houses a great diversity of molecular species. Among them, water is present in a large number of environments: from dense clouds to planetary atmospheres and comets. The tail of the latter is also supposed to contain dimers that might influence the production of ionic species [1].

However, mechanisms and kinetics of the aggregation first steps are not yet completely understood, especially at low temperature. One of the CRESU [2] set-up developed in Rennes is dedicated to study this process [3]. It couples ionization and time-of-flight mass spectrometry [4] and has already shown interesting preliminary results with water clusters (see Figure 1) and small hydrocarbons. These studies will lead to a better understanding of the dimerization processes and their potential involvement in the interstellar medium as well as in the cold planetary atmosphere (e.g. Titan).



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Présentation par affiche
Poster n° 56

Chemical modeling of high-mass star forming regions.

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In order to study the time evolution of hot cores and further stages of high-mass star forming regions, we have developed a chemical code (*Saptarsy*, Choudhury et al., 2014) which is currently working together with a radiative transfer code (RADMC3D, http://www.ita.uni-heidelberg.de/~dullemond/software/radmc-3d/). Saptarsy is a gas-grain code taking into account heavy radical movements at elevated grain temperatures (Garrod et al., 2008).

RADMC3D is first used to compute a self-consistent dust temperature profile. Secondly Saptarsy uses it as well as a density profile and a luminosity functions for accreting high-mass protostars (Hosokawa & Omukai, 2009). What we obtain at the end thanks to RADMC3D are time-dependent synthetic spectra, which will then be compared to observations, using the detail modeling of the spatio-temporal evolution of chemical abundances.

The effect of UV photons is major in those regions when a HII region starts to form. Indeed they create internals PDRs at the interface between the HII region and the molecular gas. This needs to be investigated particularly in the context of ionized flows (Krumholz et al. 2007, Peters et al. 2010) or PDRs on outflow cavities (Visser et al. 2012). The spatio-temporal evolution of the radiation field is thus currently implemented in the model in order to get a more accurate photochemistry.

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Présentation par affiche
Poster n° 57

The effects of two internal rotations in the microwave spectrum of ethyl methyl ketone.

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Ethyl methyl ketone $\mathbf{CH_3}CH_2CO\mathbf{CH_3}$ is of interest for astrophysics, since it is a potential candidate to be observed in the interstellar medium. This molecule has already been investigated very early in 1969 by Pierce *et al.* but only rotational transitions in the vibrational ground state and only the internal rotation of the acetyl methyl group -CO$\mathbf{CH_3}$ were reported [1]. Twenty years later, Pozdeev *et al.* determined the barrier to internal rotation of the ethyl methyl group $\mathbf{CH_3}CH_2CO$-, also obtained from measurements in the microwave region [2]. The higher barrier of the ethyl methyl group could only be determined from very few resolvable splittings of some transitions in the ground state with high *J* and high *K* quantum numbers. Recently, new data of ethyl methyl ketone were recorded in the microwave and millimeter-wave regions from 8 GHz to 1 THz. However, also in that work only the internal rotation of the lower-barrier acetyl methyl group was studied [3]. Using two molecular beam Fourier transform microwave spectrometers in Aachen both, the torsional fine structure with all five rotational-torsional species arising from two inequivalent methyl groups could be fully resolved and analyzed in a global fit using the BELGI-Cs-2Tops and XIAM. Molecular parameters like the rotational constants and the centrifugal distortion constants were determined with very high accuracy. The acetyl methyl group has a relatively low barrier to internal rotation causes splittings up to 1.2 GHz in the spectrum. Splittings due to the internal rotation of the ethyl methyl group are much smaller, in the order of a few hundred MHz up to 4 MHz. We found that for this molecule, the program BELGI-Cs-2Tops is much more suitable to analyze the spectrum compared to the XIAM code. For the first time, the spectroscopic work was supplemented by quantum chemical calculations for this molecule. On the other hand, quantum chemical calculations were validated by rotational spectroscopy [4].

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Présentation par affiche
Poster n° 58

The B11244 Story: C_3H^+ and C_3H^- Revisited

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Pety et al. [1] reported the first detection of the linear C_3H^+ cation in the interstellar medium toward the Horsehead photo-dissociation region. Huang et al. [2] used a perturbational approach to calculate spectroscopic parameters of C_3H^+ from a quartic internal coordinate force field. On the basis of large discrepancies between their calculated centrifugal distortion constants and those derived by Pety et al. [1], Huang et al. questioned the attribution of the transition at 11244 MHz to C_3H^+. Shortly after Fortenberry et al. [3] suggested C_3H^- as a more viable candidate for the B11244 carrier based on their quantum chemical study of this anion. The theoretical conclusions of Huang et al. [2] and Fortenberry et al. [3] triggered an additional search in interstellar environments in the context of both C_3H^+ and C_3H^- [4,5]. No observational evidence was found for the anion C_3H^-. The first laboratory confirmation of C_3H^+ as the B11244 carrier is due to Brünken et al. [6]. Botschwina et al. [7] reinvestigated the rotational parameters of C_3H^+ from the quantum chemical point of view.

In this work, the quartic force fields developed for C_3H^+ by Huang et at. [2] and for C_3H^- by Fortenberry et al. [3] are both used in combination with a numerically exact quantum mechanical method involving no dynamical approximation and no re-expansion of the potential energy contribution. Our results clearly show that the conclusions of [2,3] are not sustainable and that the perturbational approach is not sufficient to illuminate relevant spectroscopic properties. The characterization of molecular species by theoretical means is additionally reviewed, with special reference to the quasi-linear molecules (such as HCCN).

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Présentation par affiche
Poster n° 59

Ion-Molecule Reactions Involving HCO^+ and N_2H^+: Isotopologue Equilibria from New Theoretical Calculations and Consequences for Interstellar Isotope Fractionation

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The dynamics of basic isotope exchange reactions involved in the $^{12}C/^{13}C$, $^{16}O/^{18}O$, and $^{14}N/^{15}N$ balance is revisited by theoretical means [1]. We employed electronic structure methods to explore potential energy surfaces, full-dimensional numerically exact quantum mechanical approaches to compute rotational-vibrational energies, and chemical network models to estimate the abundance ratios under interstellar conditions. New exothermicities, derived for HCO^+ reacting with CO, provide rate coefficients markedly different from previous theoretical values in particular at low temperatures, resulting in new abundance ratios relevant for carbon chemistry networks. Specifically, we predict a reduction in the abundance of $H^{12}C^{18}O^+$ and an increase in the abundance of $H^{13}C^{16}O^+$ and $D^{13}C^{16}O^+$.

To gain a first insight into dynamical features of ion-molecule reactions, the ions HCO^+, HOC^+, and N_2H^+ reacting with CO and N_2 were studied. In all these cases, the reactions proceed through intermediate linear proton-bound complexes found to be very stable (bound by 2000–7000 cm^{-1}). The complexes $OCH^+\cdots CO$ and $OCH^+\cdots N_2$ have sizeable dipole moments (2.9-3.5 D) and rotational constants of approximately 2000 MHz. Vibrational frequencies and dissociation energies were additionally calculated for the proton-bound complexes $OCH^+\cdots CO$, $OCH^+\cdots OC$, $COHOC^+$, $N_2\cdots HCO^+$, $N_2H^+\cdots OC$, and $N_2HN_2^+$.

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Présentation par affiche
Poster n° 60

Spectroscopy of astrophysical molecules containing internal rotors

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Many organic compounds with internal rotation have been assigned and detected in the interstellar space. The identification of most of those molecules was based on intense laboratory work followed by observations in the interstellar medium by means of microwave, (sub)millimeter-wave telescopes. In this poster we report on the recent laboratory spectroscopic work on the methyl acetate molecule CH_3COOCH_3 and its subsequent first detection in space using the IRAM 30-m telescope [1]. The challenge of analyzing the spectra of methyl acetate is the internal rotation of two inequivalent methyl groups with one low (102.413(20) cm^{-1}) and one intermediate barrier (424.580(56) cm^{-1}) which results into a splitting of the energy levels and into five transitions (AA, AE, EA, and EE (E_3 and E_4) of symmetry species).

The poster will also show results on another non-rigid molecule, dimethyl sulfide CH_3SCH_3 (DMS) whose astronomical detection is considered as possible. DMS has two equivalent internal rotors with internal rotation barriers of about 720 cm^{-1}. The microwave spectrum of the DMS molecule has been re-measured in the 2-40 GHz frequency range, using two spectrometers in Aachen [2], with an instrumental uncertainty of a few kHz for unblended lines. A part of the millimeter spectra has been also measured for the first time in the 50-110 GHz range using the millimeter spectrometer in Aachen with an uncertainty of 40 kHz.

A fit including the new measurements and previous transitions from the literature [3] for the ground torsional state $v_t = 0$ has been performed using two different theoretical models and codes (the XIAM and the BELGI codes). The far-infrared spectrum has also been recorded for the first time at high resolution using the Fourier-transform spectrometer and the newly built cryogenic cell at the French SOLEIL synchrotron [4]. The assignments for the $v_t=1 \leftarrow 0$ torsional band under course will be presented and discussed in the poster.

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Présentation par affiche
Poster n° 61

Methylcyanobutadiyne (CH_3-C≡C-C≡C-C≡N) and Pentadiynal (H-C≡C-C≡C-CH=O): two compounds of interest for the Interstellar Medium

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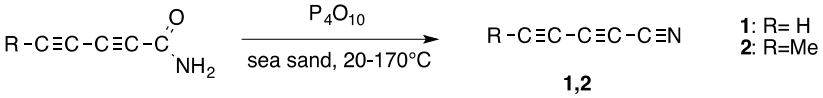
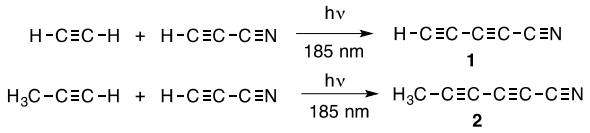
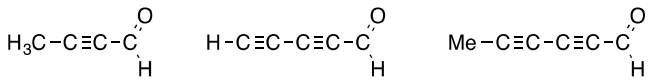
Among the about 180 molecules detected in the Interstellar Medium (ISM), the cyanopolyynes (H-(C≡C)$_n$-CN) (n=1-5) constitute the most abundant family. The methylated derivatives corresponding to the two simplest derivatives (Me-(C≡C)$_n$-CN) (n=1-2) have also been observed in the ISM. Although the first element of each series are easily synthesized in lab conditions, the two derivatives bearing two CC triple bonds are more challenging to form and the first preparation on gram-scale has been reported quite recently by our lab.[1,2]



The synthesis of such compounds in the ISM could proceed by addition of the CN radical on the corresponding alkyne as proposed by Kaiser.[3] Thus we performed some photochemical studies to show the presence of compounds **1** and **2** in various mixtures of gases and under UV irradiation at 185, 193 or 254 nm. [1,2]



On the other hand, on the basis of the huge abundance of carbon monoxide in the ISM and the detection of propynal,[4] we thought that series of aldehydes similar to the ones of cyanopolyynes could be present in the interstellar medium. We thus investigate the synthesis of the corresponding derivatives in the aim to record their microwave spectra as a tool to detect them in the ISM if they are present in this medium. The first results will be presented.



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Présentation par affiche
Poster n° 62

Interaction of Oxygen (X,^{3}P) atom with graphenic-like surfaces for astrophysical applications

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In the interstellar medium (ISM), dust grains play a key role in mediating the formation of molecular species. In order to understand and quantitatively describe the related reactive processes, it is of a strong interest to study the interactions (and reactions) of H, C, O atoms present in the interstellar clouds with (and at) grain surfaces.

Many studies have been devoted to the adsorption of hydrogen atoms, the most abundant atomic species in interstellar clouds, and to the formation of H_2 by H recombination/abstraction processes onto the surface of carbonaceous dust grains. We have shown that the atomic adsorption characteristics (physisorption/chemisorption wells, adsorption barrier, defects) play a major role in the molecular formation [1], [2].

In the ISM, the oxygen is the third abundant element after H and He. The atomic oxygen is implied in the formation of heavier molecules such as OH [3], H_2O. In this context, we have studied the adsorption of the atomic oxygen in the fundamental state ^{3}P on a carbonaceous grain. Indeed previous works have been mainly devoted to the singlet state and only a few to the triplet state [4] [5].

Our theoretical studies have been performed by means of spin polarized DFT/GGA or hybrid calculations with dispersion. The grain surface is modeled either as a graphene sheet or as PAH molecules ($C_{24}H_{12}$, $C_{54}H_{18}$). We have considered several adsorption sites: on top of a C atom of the surface, bridged between 2 adjacent C atoms of the surface.

We have obtained adsorption energies and geometries in agreement with previous works [4] [5]. The chemisorption characteristics are site dependent. Regardless of the surface considered, the more stable chemisorption site is the top site.

At larger surface-oxygen distances, the physisorption of the atomic oxygen in the ^{3}P state onto graphenic surfaces is also obtained. Depending on the surface, the physisortion characteristics are weakly site dependent.

All these electronic/structural studies, including relaxation of surrounding carbon atoms, are the first step needed for the study of the OH/H_2O formation dynamics in order to obtain reaction probabilities, energy sharing between the nascent molecules and the surface.

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Présentation par affiche
Poster n° 63

Etude photochimique de la molécule de propionitrile dans des conditions simulées de l'atmosphère de Titan

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Durant cette présentation, nous présenterons les résultats obtenus durant la photolyse à haute énergie (λ>120 nm) de la molécule de propionitrile (CH_3CH_2CN) lors de notre tentative de simulation de la photochimie atmosphérique à haute altitude sur Titan, le plus gros satellite de Saturne. Nous nous intéressons à cet astre puisque c'est le seul satellite du système solaire à posséder une atmosphère dense principalement composée de diazote (à plus de 98%). C'est pour ces raisons que les exobiologistes considèrent le cas de Titan comme analogue à la Terre primitive.

La molécule de propionitrile a été détectée sous forme solide dans la stratosphère de Titan (entre 40 et 320 kilomètres) [1] grâce à l'instrument IRIS (*Infrared Radiometer Interferometer and Spectrometer)*. Nous avons employé le principe du piégeage en matrice cryogénique de gaz rare afin de simuler la chimie atmosphérique de l'atmosphère de Titan. Dans le but de reproduire d'un point de vue énergétique le flux solaire qui atteint l'atmosphère du satellite et qui interagit avec les molécules présentes, nous avons utilisé une lampe à flux d'hydrogène (λ>120 nm) afin de photo-dissocier notre molécule de départ. L'identification des produits formés se fait par spectrométrie IRTF que nous comparons avec les calculs des spectres théoriques des molécules dont nous avons envisagé la formation.

Lorsque le propionitrile est photolysé à haute énergie (λ>120 nm), différentes voies de photodissociation ont été mises en évidence. Des composés telles que l'éthylène (C_2H_4), l'acétylène (C_2H_2), l'acide cyanhydrique (HCN) et l'acide isocyanhydrique (HNC). Nous avons également noté la formation d'acrylonitrile (CH_2CHCN) et de cyanoacétylène (HC_3N). Tous ces composés ont été détectés dans l'atmosphère de Titan et nous pouvons des hypothèses quant à leur formation à partir du propionitrile présent dans cette atmosphère.

Le fait d'effectuer ces expériences en matrice cryogénique de gaz rare nous permet d'observer des composés qui ne sont pas stables à température ambiante telles que des isonitriles c'est-à-dire que l'on observe une inversion du groupement CN terminal: nous avons noté la présence d'isoacrylonitrile (qui peut être dû à la photolyse de l'acrylonitrile formé [2]) et d'isopropionitrile.

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Can interstellar benzene be formed in a simple neutral-neutral reaction?

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Benzene, the simplest closed-shell aromatic ring, is likely to be a key primary reactant in PAH chemistry and it has been detected in circumstellar envelopes, [1] Titan's atmosphere [2] as well as in many combustion studies; thus, many reactions have been postulated to explain its formation. It is vital to investigate critical ring-forming reactions to understand PAH generation. Recently, Jones et al. [3] have reported crossed molecular beam experiments combined with electronic structure and statistical calculations to show that benzene can be synthesized via the barrierless, exoergic reaction of the ethynyl radical and 1,3-butadiene, $C_2H + H_2CCHCHCH_2 \rightarrow C_6H_6 + H$, under single collision conditions.

In order to test this proposal we have probed the products formed in the reaction of C_2H radicals with 1,3-butadiene at 4 Torr and 298 K using photoionization time-of-flight mass spectrometry. The reaction takes place in a slow-flow reactor, and products are ionized by tunable vacuum-ultraviolet light from the Advanced Light Source. The principal reaction channel involves addition of the radical to one of the unsaturated sites of 1,3-butadiene, followed by H-loss to give isomers of C_6H_6. The photoionization spectrum of the C_6H_6 product indicates that fulvene is formed with a branching fraction of (60 ± 10)%. At least one more isomer is formed, which is likely to be one or more of 3,4-dimethylenecyclobut-1-ene, 3-methylene-1-penten-4-yne or 3-methyl-1,2-pentadien-4-yne. An upper limit of 30% is placed on the branching fraction of benzene. This newly discovered cyclisation reaction yielding the 5-membered ring compound fulvene will be discussed in the context of the formation of complex organic molecules in space.

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