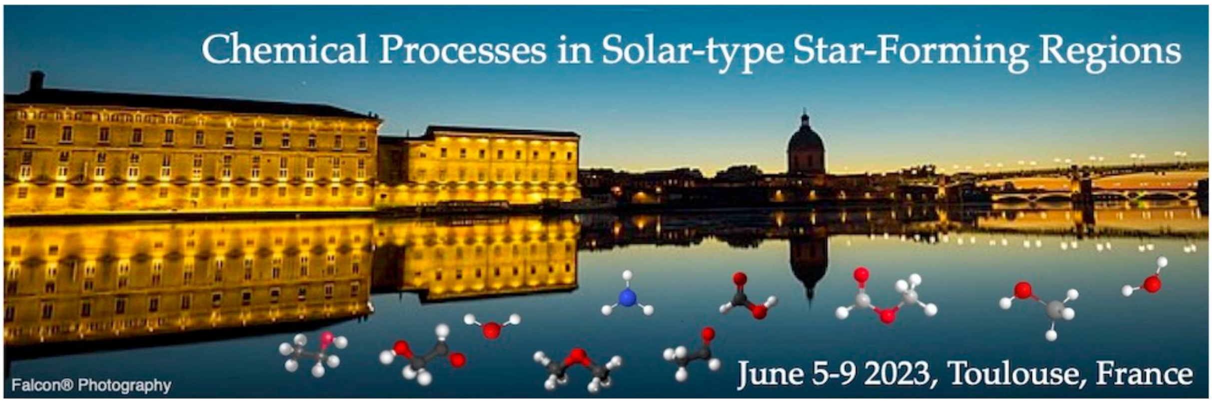


Chemical Processes in Solar-type Star-Forming Regions

June 5-9 2023, Toulouse, France

Falcon® Photography

Book of Abstract

How the chemical complexity evolves during the process leading to the formation of a Sun and its planetary system? Is the chemical richness of a Solar-like planetary system, at least partially, inherited from the earliest stages or is there a complete chemical reset?

A powerful way to answering these questions is by comparing the chemical content in young protostars and primitive bodies of the Solar System, using astrochemistry as a tool. Yet, to do so, we need to fully understand the processes that govern the chemical evolution of a molecular cloud into a young planetary system.

The goal of the conference is to gather together the actors of this intrinsically interdisciplinary endeavor: instrumentalists, astronomers, chemists and modelers.

Program of the conference “Chemical Processes in Solar-type Star-Forming Regions”

Hotel Mercure Compans Caffarelli
Toulouse (France), June 5-9 2023

(In **bold**, the invited speakers)

Monday, June 5, 2023

TIME	**EVENT**
11:00 - 13:30	Registration
13:30 - 13:50	Opening talk
Astrophysical Ices: chairman François Dulieu	
13:50 - 14:30	*The Role of Molecular Simulation in Astrochemistry* - **Piero Ugliengo**
14:30 - 14:50	*Astrochemical models of interstellar ices: history matters* - Valentine Wakelam
14:50 - 15:10	*A machine-learning model to predict the composition and temperature of infrared ice spectra* - Andrés Megías
15:10 - 15:30	*Theoretical Modeling of Olivine Clusters and of Their Interaction with Sulphur Bearing Species* - Jessica Perrero
15:30 - 16:30	**Coffee break and Poster Session**
16:30 - 17:10	*The Chemical Composition of Comets* - **Steve Charnley**
17:10 - 17:30	*A systematic comparison between molecular abundances in comets and protoplanetary disks* - Manuela Lippi
17:30 - 17:50	*Water Reactivity On Schreibersite: From Phosphites To Phosphates* - Marta Corno
17:50 - 18:00	*Presentation of Virtual reality ACO project* - Claudio Codella

Tuesday, June 6, 2023

TIME	**EVENT**
	Astrophysical Ices: chairwoman Nadia Balucani
09:00 - 09:40	*Interstellar Ices in Regions of Star Formation* - **Alexander Tielens**
09:40 - 10:00	*Comprehensive Quantum Chemistry Approach for the Evaluation of Binding Energies on Interstellar Ices. From the Water Dimer to Far-Reaching Surfaces* - Giulia Bovolenta
10:00 - 10:20	*Computed Binding Energies and Frequencies Distribution of Relevant S-Bearing Species at Interstellar Icy Grains* - Vittorio Bariosco
10:20 - 11:10	Coffee break and Poster Session
11:00 - 11:20	*Cosmic-ray-driven processes in astrophysical ices: Experimental insights* - Alexei Ivlev
11:20 - 11:40	*Formation of CO_2 on Interstellar H_2O Ice: A Computational Study* - Harjasnoor Kakkar
11:40 - 12:00	*Hydrogenation of species on water icy mantles: insights on energy dissipation from ab-initio molecular dynamics* - Stefano Pantaleone
12:10 - 14:00	**Lunch**
	Astrophysical Ices: chairwoman Cecilia Ceccarelli
14:00 - 14:20	*Revealing the chemical and dynamical history of Solar-type protostars: the crucial role of cm wavelengths* - Marta De Simone
14:20 - 14:40	*Dissipation of the Nascent Reaction Energy of Formamide Formation Route on Interstellar Water Ice Surfaces* - Berta Martínez Bachs
14:40 - 15:00	*The Role Of Low-Energy (< 20 eV) Electrons In Astrochemistry* - Christopher Arumainayagam
15:00 - 15:20	*Interstellar Ices Formation And Interaction With Molecules Of Astrochemical Interest: An In Situ Infrared Study* - Guillermo Escolano Casado
15:20 - 16:20	**Coffee break and Poster Session**
16:20 - 17:00	*Diffusion and sublimation of ices on comets and (icy)moons* - **Stéphanie Cazaux**
17:00 - 17:20	*Laboratory constraints on thermal desorption of astrophysical ice analogues* - Franciele Kruczkiewicz
17:20 - 17:40	*Sticking Coefficients of Astrochemically-Relevant Ices on Realistic Grains Analogues are Lower than Expected* - Caroline Stadler
17:40 - 18:00	*Unlocking the Interaction of CN Radical with Interstellar Ices: An Atomistic View of Polar and Apolar Environments* - Joan Enrique Romero

Wednesday, June 7, 2023

TIME	EVENT
Molecular complexity: chairman ?	
09:00 - 09:40	*Molecular complexity in Solar-System analogs* - **Eleonora Bianchi**
09:40 - 10:00	*A Challenging Quest to Unveil the Beyond-the-Second-Period Chemistry in Space* - Matteo Michielan
10:00 - 10:20	*Astrochemical Modeling of Protostellar Core Envelopes* - Prasanta Gorai
10:20 - 11:10	**Coffee break and Poster Session**
11:10 - 11:30	*Comparing the Reactivity of HCN and* $HCONH_2$ *on Amorphous and Crystalline* Mg_2SiO_4 *Surfaces: Insights into Interstellar Dust Grain Chemistry* - Rosangela Santalucia
11:30 - 11:50	*Chemical evolution during the formation of a FHSC: the B1b-N case* - David Navarro-Almaida
11:50 - 12:10	*Chemical environment of emerging hot cores: the early warm-up phase chemistry* - Laure Bouscasse
12:10 - 14:00	**Lunch**
Molecular complexity: Claudio Codella	
14:00 - 15:40	*Solid Interstellar Radical Chemistry (SIRC)* - **Fabrice Duvernay**
14:40 - 15:00	*Computational Approach for the High-Throughput Screening of Molecular Interactions for Prebiotic Astrocatalysis* - Eric Mates-Torres
15:00 - 15:20	*Constraining the diffuse envelope surrounding L1544* - Judit Ferrer Asensio
15:20 - 15:40	*Grain growth in star formation* - Pierre Marchand
15:40 - 16:40	**Coffee break**
16:40 - 17:00	*Ion-neutral reactions for formation and destruction of interstellar Complex Organic Molecules* - Daniela Ascenzi
17:00 - 17:20	*Gas-Phase Formation Of Interstellar Methyl Cyanide: Review And New Theoretical Calculations* - Lisa Giani
17:20 - 17:40	*Formation and elongation of polyglycine via unimolecular reaction in the gas phase* - Paul Bertier
17:40 - 18:00	*OMC-2 FIR4: a protostellar cluster full of surprises* - Layal Chahine
20:00 - 23:00	**Social Dinner at "Les Pieds sous la table"**

Thursday, June 8, 2023

TIME	EVENT
Molecular fractionation: chairman Alexei Ivlev	
09:00 - 09:40	*Molecular fractionation from clouds to planetary systems* - **Eva Wirström**
09:40 - 10:00	*First ALMA maps of cosmic-rays ionization rate in high-mass star-forming region* - Giovanni Sabatini
10:00 - 10:20	*A high HDO/H2O ratio in the Class I protostar L1551 IRS5* - Audrey Andreu
10:20 - 11:20	**Coffee break and Poster Session**
11:20 - 11:40	*Formaldehyde In The Dynamic Protobinary System [BHB2007] 11: Small Scale Deuteration And Large Scale Kinematics* - Lucy Evans
11:40 - 12:00	*A study of the ^{13}C and ^{15}N fractionation in low-mass starless cores* - Sigurd Jensen
12:00 - 12:20	*Formaldehyde deuteration in the young disk of IRS 63: the astrochemical link to the origin of the Solar System* - Linda Podio
12:20 - 14:00	**Lunch**
14:00 - 14:40	*Chemical evolution from molecular clouds to star-forming regions, and beyond* - **Yashiro Oba**
Molecular complexity: chairman Patrice Theulé	
14:40 - 15:00	*Combined hydrodynamic and gas-grain chemical modeling of star- forming cores* - Melisse Bonfand
15:00 - 15:20	*Heterogeneous Astrocatalysis. Mechanistic Studies For The Catalytic Formation Of iCOMs Based On Fischer-Tropsch Processes* - Gerard Pareras
15:20 - 15:40	*Hydrogenation products of CO, H_2CO and CH_3CHO, alongside NO in the interstellar medium* - Julie Vitorino
15:40 - 16:40	**Coffee break and Poster Session**
16:40 - 17:00	*Origin of COMs towards hot cores selected from ALMA-IMF* - Timea Csengeri
17:00 - 17:20	*Unravelling The Path to Molecular Complexity With Quantum Chemistry* - Isabelle Fourré
17:20 - 17:40	*Unveiling chemical structures of star-forming regions with machine learning techniques* - Katharina Giers
17:40 - 18:00	*A Spatially Resolved map of Cosmic Ray Ionization Rate and Electron Fraction* - Jaime Pineda

Friday, June 9, 2023

TIME	**EVENT**
Molecular complexity: chairwoman Christine Joblin	
09:00 - 09:20	*The chemical composition of solar-type protostars with the ALMA large spectral surveys PILS and COMPASS* - Audrey Coutens
09:20 - 09:40	*Dimerization of HCN on Interstellar Silicates Grain Cores: A Quantum Mechanical Study* - Niccolò Bancone
09:40 - 10:00	*Collision Induced Dissociation of Water Pyrene Molecular Clusters* - Arya Nair
10:00 - 10:20	*Where Planetary Systems Are Born Matters: The Chemistry Of Clustered Versus Isolated Environments And Cradle Of The Sun* - Mathilde Bouvier
10:20 - 10:40	*Astrochemically Relevant H-Atom-Abstraction and H-Atom-Addition Reactions Connecting Fulminic Acid (HCNO) and Formaldoxime (H_2CNOH)* - Barbara Keresztes
10:40 - 11:20	**Coffee break**
11:20 - 11:40	*Protostellar shocks as factories of organic molecules: the case of L1157* - Ana Lopez Sepulcre
11:40 - 12:00	*Super-Oxygenation of Naphthalene: The break-Down Reaction* - Dario Campisi
12:00 - 12:20	*The effect of metallicity on the abundances of molecules in protoplanetary disks* - Rodrigo Guadarrama
12:20 - 14:00	**Lunch**

TALKS

The Role of Molecular Simulation in Astrochemistry

Piero Ugliengo

University of Torino, Department of Chemistry, Via P. Giuria 7, Torino – ITALY

e-mail: piero.ugliengo@unito.it

There are three pieces that make up the mosaic of astrochemistry: observations, experiments in terrestrial laboratories and numerical models of the evolution of chemical species. On the other hand, the mosaic is not complete without including molecular modelling based on different degrees of approximation to the rigorous solution of the equations of molecular quantum mechanics. This piece of the mosaic has become increasingly important in recent years thanks to the impetuous development of sophisticated programs associated with powerful new computers capable of working in massively parallel mode. Thus, Dirac's paradigm, in which the fundamental laws are known but it is only a question of solving the intrinsic mathematical complexity, is being realised, at least for systems limited to 20-30 atoms. While this limitation nevertheless allows for very accurate studies of gas-phase reactivity, in the case of the simulation of interstellar grains, whether core[1] or mantle[2], the level of accuracy is necessarily lower due to two facts. The first is due to the relatively large size of the grains and the second to the amorphous, and therefore often unknown, nature of their molecular structure. Simulation is therefore a delicate balance between accuracy of calculation and adherence of the model to observational and terrestrial laboratory data, requiring experience and ingenuity. The study of solutions to these problems brings at a premium a detailed knowledge of the chemical-physical properties of the grains and their interactions with molecules of astrochemical interest, both in terms of binding energies and spectroscopically. The outcome of these calculations is essential in feeding the numerical models of chemical evolution with refined data, like kinetic constants and binding energy distribution[3]. In the talk, a summary of the recent results devoted to the molecular simulation of both core and mantle grains will be reported. For the mantle, adsorption of relevant molecules (H_2O, NH_3, CH_3OH and H_2S) will also be discussed.

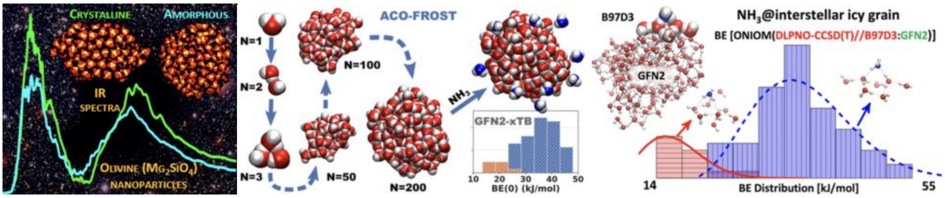


Figure 1: *Models of grain core and mantle and NH_3 binding energy distribution.*

1. L. Zamirri et al, *ACS Earth Space Chem*. **2019**, 3, 2323–2338.
2. A. Germain et al, *ACS Earth Space* Chem. **2022**, 6, 1286–1298.
3. L. Tinacci et al, *ACS Earth Space Chem*. **2022**, 6, 1514–1526.

Astrochemical models of interstellar ices: history matters

V. Wakelam [1] , A. Clément[1,2], A. Taillard[1], P. Gratier[1], JC Loison[3], E. Dartois[4], F. Dulieu[5], J. A. Noble[6], M. Chabot[7]

[1]Laboratoire d'Astrophysique de Bordeaux (LAB), Univ. Bordeaux, CNRS, B18N, allée Geoffroy Saint-Hilaire, 33615 Pessac, France

[2] Universite Bordeaux, CNRS, LP2I Bordeaux, UMR 5797, F-33170 Gradignan, France
[3] Institut des Sciences Moléculaires (ISM), CNRS, Univ. Bordeaux, 351 cours de la Libération, 33400, Talence, France
[4] Institut des sciences Moléculaires d'Orsay, CNRS, Université Paris-Saclay, Bât 520, Rue André Rivière, 91405 Orsay, France
[5] CY Cergy Paris Université, Observatoire de Paris, PSL Research University, Sorbonne Université, CNRS, LERMA, F-95000, Cergy, France
[6] Physique des Interactions Ioniques et Moléculaires, CNRS, Aix Marseille Univ., 13397 Marseille, France
[7] Laboratoire des deux infinis Irène Joliot Curie (IJClab), CNRS-IN2P3, Université Paris-Saclay, 91405 Orsay, France

e-mail: presenting valentine.wakelam@u-bordeaux.fr

Ice is ubiquitous in the interstellar medium as soon as it becomes slightly opaque in the visible, i.e. for visual extinctions (Av) above ~1.5. Observations of interstellar ices in the infrared have shown that they are mostly composed of water. CO_2 is also detected towards all lines of sight, with the exception of peculiar circumstellar environments such as around OH/IR stars where pure water ice is observed (see Boogert et al. 2015, and references therein). Other molecules, such as CO, CH_3OH, CH_4, NH_3, and H_2CO are also identified with varying amounts (between a few percent to a few tens of percent with respect to H_2O) depending on the observed environment. In cold cores, the water ice is observed for visual extinction higher than a threshold Av of approximately 1.5 (i.e. half of the observed visual extinction threshold, considering only one side of the cloud), while CO ice is seen for Av higher than 3 and CH_3OH for Av higher than 9. CO_2 ice is observed with a threshold Av similar to H_2O over all lines of sights. The James Webb Space Telescope (JWST) will observe the ice composition towards hundreds of lines of sight, covering a large range of physical conditions in these extinct regions.

In this context, we conducted a theoretical study of the chemical ice composition in a large range of cold core physical conditions in order to understand the formation of the main ice constituents and also make predictions of the sensitivity of the ice composition to the physical conditions, by considering those along the most diffuse lines of sight as well as those in the cold core (Clément et al. submitted). We start from an initial composition – gas-phase and mostly atomic – and compute time-dependent chemistry for a set of physical parameters. While doing this, we will show that more sophisticated time-dependent physical conditions that follow the formation of cold cores from the earliest stages are needed to explain the general features of observed ice.

A Machine Learning Model to Predict the Composition and Temperature of Infrared Ice Spectra

Andrés Megías,[1] Izaskun Jiménez-Serra [1]

[1] *Centro de Astrobiología (CAB), CSIC-INTA*
Carretera de Ajalvir, km 4, Torrejón de Ardoz – SPAIN

e-mail: amegias@cab.inta-csic.es

Current and future observations carried out by the James Webb Space Telescope (JWST) allow to observe the absorption features of ices along the process of star formation. Thanks to its unprecedented sensitivity and high spectral resolution, JWST has the potential to reveal the complex organic content of ices. However, identifying their ice spectral features is not trivial but a time-demanding task that is usually done manually.

In this talk I will present a machine-learning algorithm consisting of a neural network that allows us to predict the ice fractional composition and temperature of a given absorption spectrum. In order to train the neural network, we have used hundreds of laboratory experiments of ice mixtures available from the Leiden Ice Database. The algorithm is very fast and our results show a good agreement for those molecular species for which a large amount of data is available (about 3 % of error). For species with less laboratory data available, the errors are however a bit larger (of the order of 10 %).

In this contribution I will also provide examples of the fit obtained with our new neural network algorithm, of JWST ice data recently reported toward two highly-extinguished background stars (with $A_V > 50$ mag) located in the Chameleon I molecular cloud and star-forming region.

Theoretical Modeling of Olivine Clusters and of Their Interaction With Sulphur Bearing Species

Jessica Perrero[1,2], Albert Rimola[1], and Piero Ugliengo[2]

[1] *Universitat Autònoma de Barcelona, Departament de Química, E-08193, Bellaterra, – SPAIN*

[2] *Università degli Studi di Torino, Dipartimento di Chimica, I-10125, Torino – ITALY*

e-mail: jessica.perrero@uab.cat

Interstellar dust grains are irregular, micron-sized, solid aggregates of graphite and/or silicates found in the interstellar medium (ISM). Grains provide a surface where species can meet, accrete, and react. Indeed, they are thought to be responsible for most of the formation of H_2 and H_2O[1]. In diffuse molecular clouds, the mineral core of the grains can be exposed to the atoms and small molecules present in the gas phase. Sulphur depletion in the ISM is a long-standing issue, as its expected elemental abundance in dense molecular clouds cannot be achieved when considering only the species detected in the gas phase[2]. Therefore, it is our aim to understand how gas phase sulphur-bearing species interact with the grains on which OCS and, tentatively, SO_2 were observed[3]. Therefore, a better understanding of sulphur chemistry is needed, starting from its behaviour in diffuse clouds where only the core of the grains is present.

To simulate the olivine grain core, a family of silicates containing Mg and Fe and one of the most abundant minerals in the ISM, we performed a series of quantum mechanical benchmark calculations to find a suitable methodology for the characterization of their structures, represented by nanoclusters of $Mg_4Si_2O_8$ and $Mg_3FeSi_2O_8$[4].

We used H_2S to fine tune the computational methodology, extending the study to other S-bearing species. Our calculations reveal that sulphur prefers to interact with Fe rather than with Mg, and that the strength of the interaction is such that the species are likely to stick onto the mineral surfaces, becoming part of the grain core. This may, in part, account for the S-depletion in the gas-phase.

1. E.F. van Dishoeck, E. Herbst, and D.A. Neufeld, *Chem. Rev.*, **2013**, 113, 9043-9085

2. J.C. Laas, and P. Caselli, *Astron. Astrophys.*, **2019**, 624, A108

3. A.A. Boogert, P.A. Gerakines, and D.C. Whittet, *Annu. Rev. Astron. Astr.*, **2015**, 53, 541-581

4. M. Serra-Peralta, C. Domínguez-Dalmases, and A. Rimola, *Phys. Chem. Chem. Phys.*, **2022**, 24, 28381-28393

The Chemical Composition of Comets

Steven Charnley[1]

[1]*University of XXXX*, NASA/GSFC, Greenbelt, Maryland, United States
e-mail: steven.b.charnley@nasa.gov

I will summarize what is currently known of the chemistry of comets. Sublimation of nuclear ices near perihelion generates the coma - a multi fluid plasma whose understanding requires consideration of a variety of chemical processes. Compositional studies, from ground and space, especially of organic molecules, isotopologues, and ortho-para ratios can provide important clues as to their origins, and to their possible role in providing water and biomolecules to the early Earth.

1. Mumma, M. J. Charnley, S.B. (2011), Annu. Rev. Astron. Astrophys., 49, 471

A systematic comparison between molecular abundances in comets and protoplanetary disks

Manuela Lippi[1], Linda Podio[1], and Claudio Codella[1]

[1]*INAF - Osservatorio Astrofisico di Arcetri, Largo Enrico Fermi 5, I-50125 Firenze, Italy*

e-mail: manuela.lippi@inaf.it

We present a statistical comparison between molecular abundances in comets and protoplanetary disks.

Comets formed around the young Sun, about 4.6 billion years ago. Different models predict their formation at different distances from the protosun and their successive dispersion into their present reservoirs[1,2], where the comet's nuclei remained frozen, preserving most of the chemical and mineralogical properties linked to their formation site.

Indeed, comets show properties like the pre-stellar ice's ones as well as diverse features that can only be explained considering high temperature/radiation processing of the material before its incorporation in the nuclei[3].

A systematic comparison between the chemical composition measured in comets with that of planet formation regions can thus reveal key clues on the physical, chemical, and evolutionary processes in act during the formation of our and other planetary systems (e.g., hydrogenation on dust grains in cold environments or photo-dissociation processes due to UV/X-rays/Cosmic-rays radiation).

Preliminary works show possible correlations and similarities between comets and protoplanetary disks compositions[4,5,6]. We have increased and proper combined these statistics, and we will show how the relationships among simple molecules (e.g., CO, CH_3OH, H_2CO) retrieved in 30 comets and in protoplanetary disks can be used to investigate the origins of our solar system.

Work funded by Next Generation EU and PNRR – Italia Domani.

1. Gomes, R., Levison, H. F., Tsiganis, K., & Morbidelli, A., *Nature*, **2005**, 435, 466.

2. Morbidelli, A., Tsiganis, K., Crida, A., Levison, H. F., & Gomes, R., *The Astronomical Journal*, **2007**, 134, 1790.

3. Mumma, M. J. & S. B. Charnley, *Ann. Rev. Astron. Astroph*., **2011**, 49,471

4. Lippi, M., Villanueva, G. L., Mumma, M. J., & Faggi, S., *The Astronomical Journal,* **2021**, 162, 74.

5. Drozdovskaya, M. N., van Dishoeck, E. F., Rubin, M., Jørgensen, J. K., & Altwegg, K., *Monthly Notices of the Royal Astronomical Society*, **2019**, 490, 50.

6. Podio, L., Garufi, A., Codella, C., Fedele, D., Bianchi, E., Bacciotti, F., Ceccarelli, C., Favre, C., Mercimek, S., Rygl, K., & Testi, L., *Astronomy & Astrophysics,* **2020**, 642, L7.

Water Reactivity On Schreibersite: From Phosphites To Phosphates

Marta Corno[1], S. Pantaleone[1], A. Rimola[2], N. Balucani[3] and Piero Ugliengo[1]

[1]*University of Turin, Department of Chemistry, Via P. Giuria 7, I-10125 Torino – ITALY*

[2]*Universitat Autònoma de Barcelona, Departament de Química, 08193 Bellaterra, Catalonia, – SPAIN*

[3]*Università degli Studi di Perugia, Dipartimento di Chimica, Biologia e Biotecnologie, Via Elce di Sotto 8, I-06123 Perugia – ITALY*

e-mail: marta.corno@unito.it

Phosphorus is an element of primary importance for all living creatures, being present in many biological activities in the form of phosphate (PO_4^{3-}). However, open questions about its origin and transformations remain. The most probable source of prebiotic phosphorus is the meteoritic bombardment during the Archean era, delivering tons of iron-phosphide materials (schreibersite) on the early Earth crust.[1] It has been recently shown that wetting/corrosion processes on this material formed various oxygenated phosphorus compounds.[2]

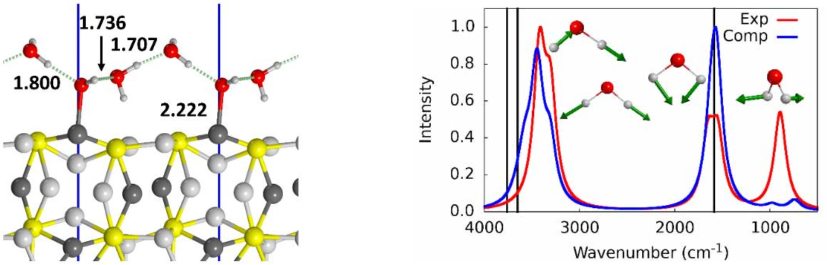


Figure 1: *H_2O monolayer on the (110) Fe_2NiP surface (left); experimental vs computed IR spectrum at 125 K (right). H in white, O in red, P in yellow, Fe in light grey, Ni in dark grey.*

In the present work, the wetting process of schreibersite (Fe_2NiP) was simulated by density functional theory, with the PBE D*0 functional, including dispersive interactions.[3,4] In detail, different water coverages on the two stable (110) and (001) Fe_2NiP surfaces have been simulated, resulting in water binding energy values and vibrational spectra prediction. The validity of the adopted approach was then confirmed by comparing computed and experimental IR spectra (Figure 1).[5] Moreover, water reactivity was inspected in several possible deprotonation reactions, also increasing the number of water molecules to lead to the formation of phosphonic and phosphoric acids and to their corresponding deprotonated forms.

1. A. Gulick, *Am. Sci.* **1955**, 43, 479-489
2. M. A. Pasek, D. S. Lauretta, *Astrobiology* **2005**, 5, 515-535
3. S. Pantaleone, M. Corno, A. Rimola, *et al.*, *ACS Earth Space Chem.* **2021**, 5, 1741-1751
4. S. Pantaleone, M. Corno, A. Rimola, N. Balucani, P.Ugliengo, *J. Phys. Chem. C* **2022**, 26, 2243-2252
5. D. Qasim, L. Vlasak, A. Pital, *et al.*, *J. Phys. Chem. C* **2017**, 121, 13645-13654

Interstellar Ices in Regions of Star Formation

A.G.G.M Tielens
Leiden Observatory & Astronomy Department University of Maryland

Infrared spectra of background stars behind dark cloud cores and of embedded protostars show prominent absorption features at 3.08, 3.54, 4.23, 4.38, 4.67, 4.9, 6.0, 6.85, 7.6 and 15.2 µm. These features are due to simple molecules such as H_2O, CH_3OH, CO_2, CO, OCS, and CH_4 at varying concentrations in accreted icy grain mantles. These studies have revealed the presence of several independent ice components, often along the same line of sight. These different components seem to be related to the effects of thermal processing by embedded protostars. Heating by embedded sources can lead to sublimation of these species into the gas phase, creating so-called Hot Corinos and Hot cores with a rich and diverse organic inventory that is linked to the outgassing ices.

These molecular ice mantles are thought to form by accretion and reaction of gas phase species on interstellar grain surfaces. Important grain surface routes will be delineated. Interstellar ices can also be processed by FUV photons. This photolysis will lead to the formation trapped radicals that may be released by thermal processing giving rise to a rich chemistry. These different chemical routes towards molecular complexity in regions of star formation will be pointed out and possible links to the solar system organic inventory will be made.

Comprehensive Quantum Chemistry Approach for the Evaluation of Binding Energies on Interstellar Ices.
From the Water Dimer to Far-reaching Surfaces

G. M. Bovolenta[1], S. Vogt-Geisse[1], S. Bovino[2]

[1]*Departamento de Físico-Química, Facultad de Ciencias Químicas, Universidad de Concepción, Av. Edmundo Larenas 129, Concepción – CHILE*

[2]*Departamento de Astronomía, Facultad Ciencias Físicas y Matemáticas, Universidad de Concepción, Av. Esteban Iturra s/n, Concepción – CHILE*

e-mail: gbovolenta@udec.cl

The quality of astrochemical models is highly dependent on reliable binding energy (BE) values that consider the morphological and energetic variety of binding sites on the surface of ice-grain mantles.

In this work, we present a comprehensive approach for the computation of the binding energy of small interstellar species on amorphous solid water (ASW) surfaces. Our approach is based on the refinement of the binding energy value on two different levels: the accuracy of the employed model chemistry and the ice surface approximation.

We propose three tiers of model surfaces. The first model is a set of small water clusters up to the tetramer, which is used to benchmark several density functional theory (DFT) methods to a highly accurate coupled cluster CCSD(T)/CBS reference, in order to choose an appropriate functional to describe the adsorbate-surface interaction. The second ASW model is spanned by a set of 15-20 amorphized 22-water molecule clusters, which allows to build a binding energy distribution[1,2,3], due to the statistical variety of unique binding sites on each cluster. Finally, we selected equilibrium structures of adsorbed molecules on a group of clusters of different sizes, to be used as a starting point to generate a balanced training set for Gaussian Moment Neural Network (GM-NN)[4] potentials, able to reproduce the adsorption site as well as the water hydrogen-bonding network, at an equivalent to coupled cluster curated hybrid-DFT/def2-TZVP level of theory. Using those *ad hoc* NN-potentials, we built a periodic model composed of five ~500-water molecule surfaces and computed highly accurate binding energy distributions. We present the results for astrophysically important CO and HCO species using the described procedure.

1. G. Bovolenta, S. Bovino, E. Vöhringer-Martinez, D. A. Saez, T. Grassi, S. Vogt-Geisse, *Mol. Astrophys*, **2020**, 100095.

2. G. M. Bovolenta, S. Vogt-Geisse, S. Bovino, T. Grassi, *ApJS*, **2022**, 262, 17.

3. `www.github.com/qcmm/beep`

4. V. Zaverkin and J. Kästner, *J. Chem. Theory Comput.*, **2020**, 16, 5410–5421.

Computed Binding Energies and Frequencies Distribution of Relevant S-Bearing Species at Interstellar Icy Grains

V. Bariosco[1], S. Pantaleone[1], A. Germain[1], L. Tinacci[2], C. Ceccarelli[2], A. Rimola[3], M. Corno[1] and P. Ugliengo[1]

[1]*University of Turin, Department of Chemistry, Via Pietro Giuria 7, Turin – ITALY*

[2] *Université Grenoble Alpes, IPAG, 414 Rue de la Piscine, Grenoble – FRANCE*

[3]*Universitat Autònoma de Barcelona, Departament de Química, 08193, Bellaterra - SPAIN*

e-mail: vittorio.bariosco@unito.it

Binding energies (BEs) are crucial parameters to understand the evolution of molecular species in dense clouds, determining whether a species is frozen onto the grain surfaces or free in the gas phase. Nowadays, BEs are usually provided as single point values, however the predominant amorphousness of icy grains gives rise to a distribution of BE sites and values. Until now, several grain models have appeared in literature, however, lacking a comprehensive physical and systematical description. Recently, ACO-FROST, an automatic procedure to simulate realistic icy grains has been released.[1] This code allows to build up models of amorphous ice up to 1000 molecules and to simulate a large variety of BE sites, see Figure 1 left panel.

In the present work, the aforementioned procedure was applied to compute BE distribution of S-bearing species, *i.e.,* H_2S, OCS, CH_3SH. S-species were selected in order to contribute to a long-standing issue in the field: the Sulphur depletion problem.[2] BEs were computed at DFT level (B97-3c) and then refined with one of the highest level of theory available (DLPNO-CCSD(T)). The previous reported BE values are overestimated with respect to our new BE distribution,[3] see Figure 1 central panel. Besides, frequencies distribution was calculated for OCS molecule and compared to the James Webb Space Telescope (JWST) observations[4] as reported in Figure 1 right panel. The computed distribution outstandingly reproduces JWST data indicating the robustness of the model studied and thus defining a novel computational tool to predict icy species vibrational features.

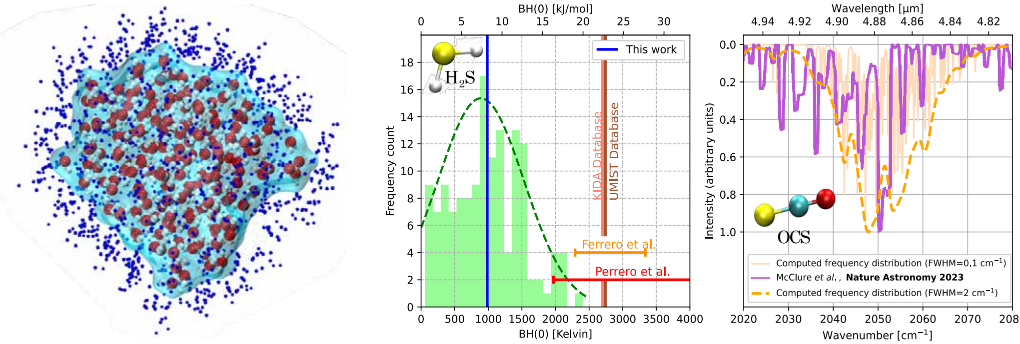


Figure 1: *Left panel: 200-H_2O grain covered by a grid of 486 BE sampling sites. Central panel: BE distribution of H_2S compared with previous results. Right panel: Computed frequencies distribution for OCS molecule compared with JWST observations.*

1. A. Germain, L. Tinacci, S. Pantaleone, *et al.*, *ACS Earth Space Chem*. **2022**, 6, 1286-1298
2. R. Martin-Domenech, I. Jimenez-Serra, G. M. M. Caro, *et al.*, *Astron. Astrophys*. **2016**, 585, 1-9
3. S. Ferrero, L. Zamirri, C. Ceccarelli, *et al.,* ApJ **2020**, 904, 1-20
4. M. K. McClure, W. R. M. Rocha, K. M. Pontoppidan, *et al., Nature Astronomy* **2023**, 1-13

Cosmic-ray-driven processes in astrophysical ices: Experimental insights

A. Ivlev[1], B. M. Giuliano[1], P. Caselli[1], S. Ioppolo[2], and Atomki Team[3]

[1] *Max-Planck-Institut für Extraterrestrische Physik, D-85748 Garching – GERMANY*

[2] *Centre for Interstellar Catalysis (InterCat), Department of Physics and Astronomy, Aarhus University, DK 8000 Aarhus – DENMARK*

[3] *Institute for Nuclear Research (Atomki), PO Box 51, H-4026 Debrecen – HUNGARY*

e-mail: ivlev@mpe.mpg.de

We present a dedicated experimental study of microscopic mechanisms controlling radiolysis and sputtering of astrophysical ices due to their bombardment by cosmic ray ions. Such ions are slowed down due to inelastic collisions with bound electrons, resulting in ionization and excitation of ice molecules. In experiments on CO ice irradiation, we show that the relative contribution of these two mechanisms of energy loss to molecule destruction and sputtering can be probed by selecting ion energies near the peak of the electronic stopping power. We have observed a significant asymmetry, both in the destruction cross section and the sputtering yield, for pairs of ion energies corresponding to same values of the stopping power on either side of the peak. This implies that the stopping power does not solely control these processes, as usually assumed in the literature. Our results suggest that electronic excitations represent a significantly more efficient channel for radiolysis and, possibly, also for sputtering of CO ice[1].

1. A. V. Ivlev, B. M. Giuliano, P. Caselli, et al., *ApJ.* **2023**, to be published (arXiv:2301.09401).

Formation of CO_2 on Interstellar H_2O Ice: A Computational Study

Harjasnoor Kakkar[1], and Albert Rimola[1]

[1] *Universitat Autònoma de Barcelona, Departament de Química, 08193, Bellaterra – SPAIN*

e-mail: harjasnoor.kakkar@uab.cat

Solid CO_2 was first detected in the interstellar medium (ISM) in 1989, and since then, has been observed in varied physical environments ranging from quiescent regions of dark clouds to massive protostars[1]. Despite being one of the most abundant species in the ISM and a significant component of ice mantles covering dust grains, the formation route of CO_2 is still under speculation[2]. The low abundance of CO_2 in the gas phase indicates that it is formed exclusively on the solid ice surface. Moreover, there is no clear, efficient process that can account for the majority of CO_2 formation[3]. In this work, we consider three well-known radical-neutral reaction pathways on pure water ice clusters: CO with O, CO with OH, and HCHO with O. Quantum chemical calculations have been carried out for the preliminary benchmarking study using multiple DFT functionals on model gas-phase reactions, to ascertain a method that accurately describes the reaction properties. With the selected functional, potential energy surfaces of the reactions are obtained on ice models i.e., two water clusters composed of 18 and 33 molecules. First insights will be presented based on the computational investigation of the reaction mechanisms to determine if they are energetically feasible. Additionally, astrophysical implications of the results will be discussed in combination with the observations from experiments and astrochemical models of these widely studied reactions.

1. J. E. Roser, G. Vidali, et al. *Astrophys. J.* **2001**, 555, L61-L64
2. M. Minissale, E. Congiu, et al. *Astron. Astrophys.* **2013**, 559, A49
3. R. T. Garrod, T. Pauly. *Astrophys. J.* **2011**, 735, 15

Hydrogenation of species on water icy mantles: insights on energy dissipation from ab-initio molecular dynamics

S. Pantaleone[1], S. Ferrero[2], J. Enrique-Romero[2], C. Ceccarelli[4], N. Balucani[5], A. Rimola[2], P. Ugliengo[1]

[1]*Università degli Studi di Torino, Dipartimento di Chimica and Nanostructured Interfaces and Surfaces (NIS) Centre, via P. Giuria 7, Torino - Italy*

[2]*Universitat Autònoma de Barcelona, Departament de Química, Bellaterra – Spain*

[4]*Univ. Grenoble Alpes, CNRS, Institut de Planétologie et d'Astrophysique de Grenoble (IPAG), Grenoble - France*

[5]*Università degli Studi di Perugia, Dipartimento di Chimica, Biologia e Biotecnologie, Via Elce di Sotto 8, Perugia - Italy*

e-mail: stefano.pantaleone@unito.it

Molecular clouds are the cold regions of the Milky Way where stars form. They are enriched by rather complex molecules.[1,2] Many of these molecules are believed to be synthesized on the icy surfaces of the interstellar submicron-sized dust grains that permeate the Galaxy.[3] At 10 K thermal desorption is inefficient and, therefore, why these molecules are found in the cold gas has tantalized astronomers for years. The assumption of the current models, called chemical desorption, is that the molecule formation energy released by the chemical reactions at the grain surface is partially absorbed by the grain and the remaining energy causes the ejection of the newly formed molecules into the gas.[4] Here we report *ab-initio* molecular dynamics simulations aimed at studying the dissipation energy of hydrogenation reactions: i) $H + H \rightarrow H_2$,[5] ii) $H + CO \rightarrow HCO$,[6] and iii) $N + H \rightarrow NH$, $NH + H \rightarrow NH_2$, $NH_2 + H \rightarrow NH_3$.[7] In all cases the presence of the ice mantle, acting as third body to absorb the released reaction energy (from 50 up to 90%), is mandatory to stabilize the product. In the case of H_2, the weak interaction with the surface and the large energy kept by the molecule, ensure the desorption of the species in a relatively short timescale (from 1 ns up to 1000 yr). On the contrary, both HCO and NH stay stuck on the ice surface, thus allowing for successive hydrogenation reaction to form the corresponding final products: methanol (CH_3OH) and ammonia (NH_3), respectively.

1. C. Ceccarelli, P. Caselli, F. Fontani, et al., *Astrophys. J.* **2017**, 850, 176
2. E. Herbst, E. F. van Dishoeck, *Annu. Rev. Astron. Astrophys.* **2009**, 47, 427
3. D. Hollenbach, E. Salpeter, *J. Chem. Phys.* **1970**, 53, 79-86
4. R. T. Garrod, V. Wakelam, E. Herbst, *Astron. Astrophys.* **2007**, 467, 1103
5. S. Pantaleone, J. Enrique-Romero, C. Ceccarelli, et al., *Astrophys. J.* **2021**, 917, 49
6. S. Pantaleone, J. Enrique-Romero, C. Ceccarelli, et al., *Astrophys. J.* **2020**, 897, 56
7. S. Ferrero, S. Pantaleone, C. Ceccarelli, et al., *Astrophys. J.* **2023**, 944, 142

Revealing the chemical and dynamical history of Solar-type protostars: the crucial role of cm wavelengths

De Simone Marta[1] et al.

[1]*European Southern Observatory (ESO), Karl Schwarzschild 2, Garching – GERMANY*
e-mail: marta.desimone@eso.org

The early stages of the formation of a planetary system are represented by Solar-type protostars. Recent research suggests planet formation may begin already at these stages. Thus, the chemical content of protostars can be directly linked to what future forming planets can inherit. However, protostars are far to be fully chemically characterized. Indeed, a chemical diversity in their millimeter spectra has been observed and it is not well understood yet.

The gaseous chemical content of protostars depends on the composition of the icy dust grain mantles formed before collapse begins. Directly measuring the ice mantle composition in these embedded objects is challenging, but it can be inferred indirectly by observing the ice major species once they are release into the gas phase during the warm protostellar stage.

In this contribution, I will show the results from our VLA high spatial resolution (~300 au) observations of NH_3 and CH_3OH (critical ice mantle tracers). By comparing the NH_3/CH_3OH ratio with up-to-date astrochemical models, we retrieved the chemical and dynamical history of the NGC1333 IRAS 4 protostars (the 4A binary and 4B; De Simone et al. 2022, ApJL). In summary, the three protostars share the same history, characterized by a rapid collapse triggered by a brutal external event (De Simone et al. 2022, MNRAS), which set the observed chemistry. These findings highlight the crucial role of centimeter observations in retrieving i) the dust contribution in absorbing the molecular emission, ii) the protostellar ice mantle history, and iii) the dynamics of the protostars' birth environment.

Additionally, I will show preliminary results on follow up VLA observations of the intermediate mass Cep E-mm binary protostellar system. Contrary to IRAS 4A, the companion that dominates the continuum possess a hot corino region detectable at mm wavelengths, while the fainter does not. Is the dust still responsible for the observed diversity? What is the chemical history behind this system?

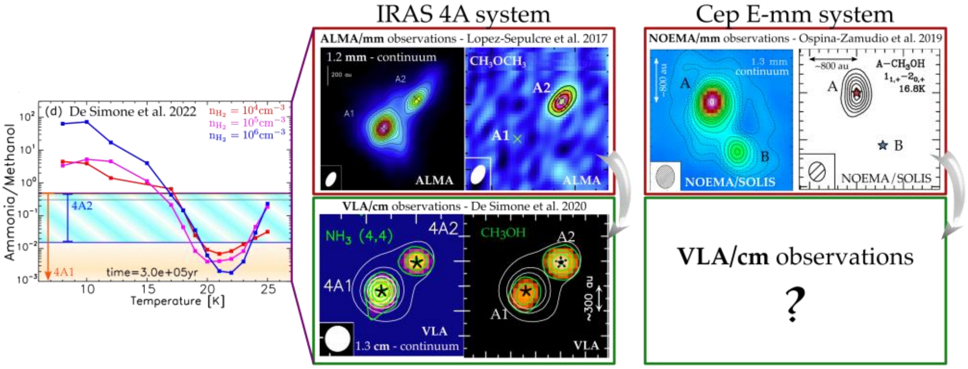


Figure 1: *Cep-E shows, at mm- wavelengths, is different from IRAS 4A with respect to having the brightest continuum source rich in iCOMs. The IRAS 4A1 hot corino was hidden by the dust and the two companion share the same chemical history. What about Cep E-mm?*

Dissipation of the Nascent Reaction Energy of Formamide Formation Route on Interstellar Water Ice Surfaces

Berta Martínez-Bachs[1] , Gerard Pareras[1], Joan-Enrique Romero[2] and Albert Rimola[1]

[1]*Universitat Autònoma de Barcelona, Departament de Química, 08193 Bellaterra, Spain*

[2]*Leiden Institute of Chemistry, Leiden, University, Leiden 2300 RA, The Netherlands*

e-mail: berta.martinez@uab.cat

Ice mantles covering dust particles provide a solid-state support for chemical reactions in the Interstellar Medium. Such water ice surfaces can act as third bodies by absorbing the energy released by surface reactions[1]. Indeed, the absorbing capacity of ice mantles is a crucial factor that will determine if newly formed species on their surfaces will remain adsorbed on the ices or will be desorbed and ejected into the gas-phase as it is commonly assumed by astrochemical models[2, 3]. In this contribution, we analyze the third-body role of water ice mantles for the radical-radical coupling between NH_2 and HCO to form formamide, a reaction that presents a low energy barrier and is largely exothermic[4]. Its potential energy surface has been characterized on an amorphous water ice model using static quantum chemical methods. Ab initio molecular dynamics simulations have been performed to elucidate how the nascent reaction energy is dissipated through the amorphous water ice model. Results indicate that water ices present a high absorbing capacity and, therefore, the energy that remains on the newly formed formamide is not large enough to cause its ejection into the gas-phase.

1. A. Potapov and M. McCoustra, Int. Rev. Phys. Chem., 2021, 40, 299-364

2 S. Pantaleone, J. Enrique-Romero, C. Ceccarelli, P. Ugliengo, N. Balucani, and A. Rimola, Astrophys. J., 2020, 897, 56-68

3. S. Pantaleone, J. Enrique-Romero, C. Ceccarelli, S. Ferrero, P. Ugliengo, N. Balucani, and A. Rimola., Astrophys. J., 2021, 917, 49-59

4. J. Enrique-Romero, A. Rimola, C. Ceccarelli, P. Ugliengo, N. Balucani, and D. Skouteris, ACS Earth Space Chem., 2019, 3, 2158-2170

The Role Of Low-Energy (< 20 eV) Electrons In Astrochemistry

Christopher Arumainayagam[1], Qin Tong Wu[1], James Battat[2], and Marco Padovani[3]

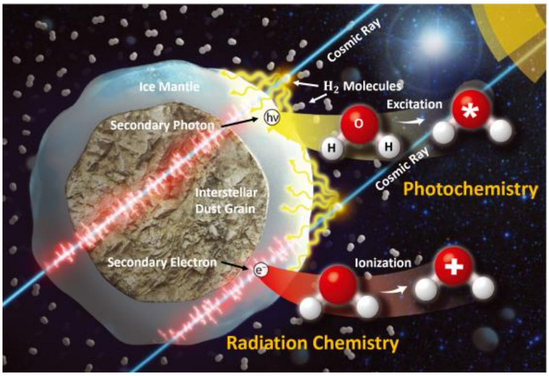
[1]*Wellesley College, Department of Chemistry, 106 Central St, Wellesley – USA*

[2]*Wellesley College, Department of Physics, 106 Central St, Wellesley – USA*

[3]*INAF—Osservatorio Astrofisico di Arcetri, 5 Largo E. Fermi, Firenze – Italy*

e-mail: carumain@wellesley.edu

Radiation chemistry and photochemistry inside the ice mantles surrounding micron-size dust grains within dark, dense molecular clouds likely dominate the synthesis of prebiotic molecules (e.g., glycine) in the interstellar medium[1]. We explore the relative importance of low-energy (<20 eV) secondary electrons — instigators of radiation chemistry — and low-energy photons (<10 eV) — instigators of photochemistry. We estimate the flux of cosmic-ray-induced secondary electrons within interstellar ices by 1) considering the attenuated cosmic-ray particle spectra after propagation through dark, dense molecular clouds and 2) incorporating data from the National Institute for Standards and Technology (NIST) databases to account for the total stopping power (the energy loss per unit length) for particles in liquid water. Photons produced via excitation of gaseous hydrogen within dense molecular clouds have a flux of ~10^3 photons cm^{-2} s^{-1} whereas our order-of-magnitude calculations indicate fluxes as high as ~10^2 electrons cm^{-2} s^{-1} for low-energy secondary electrons produced within interstellar ices due to incident cosmic rays. Furthermore, reaction cross-sections can be several orders of magnitude larger for electrons than for photons because (1) electron-induced singlet-to-triplet transitions are allowed, (2) electrons can be captured into resonant negative ion states that may then dissociate[2] (3) electron impact excitation is not a resonant process. Therefore, our laboratory studies and order-of-magnitude calculations suggest that the role of low-energy secondary electrons is at least as significant as that of photons in the interstellar synthesis of prebiotic molecules, which likely seeded Earth via comets and meteorites in a process referred to as molecular panspermia.



1. C. Arumainayagam, R. Garrod, M. Boyer, A. Hay, S. Bao, J. Campbell, J. Wang, C. Nowak, M. Arumainayagam, P. Hodge, *Chem. Soc. Rev*. **2019**, 48, 2293-2314

2. C. Aruminaygam, H. Lee, R. Nelson, D. Haines, R. Gunawardane, *Surf. Sci. Rep*. **2010**, 1, 1-44

Interstellar Ices Formation And Interaction With Molecules Of Astrochemical Interest: An *In Situ* Infrared Study

Guillermo Escolano-Casado[1], Rosangela Santalucia[1], Lorenzo Mino[1], Giuseppe Spoto[1], and Piero Ugliengo[1]

[1]*University of Turin, Department of Chemistry and Interdepartmental Centre NIS, Via Pietro Giuria 7, Torino – ITALY*

e-mail: guillermo.escolanocasado@unito.it

Sub-micron sized grains have been detected in the coldest (≤ 20 K) part of the interstellar medium (ISM). These interstellar grains are composed by a mineral core (silicates, carbonates, etc) embedded by a layer of adsorbed ice containing diverse volatile species (H_2O, CO_2, CO, CH_3OH, and NH_3), the so-called "dirty ices". It has been demonstrated the key role of these interstellar dust grains either in the hydrogenation of atomic species, and for the formation of iCOMs. From an experimental point of view, the simulation of the interstellar conditions is extremely challenging due to extremely low temperatures and pressure; as a consequence, the majority of these studies have been performed on ice analogues made by inert materials that cannot account for the actual interactions exerted by an interstellar ice. But the performed experimental studies simulating the ice formation conditions are scarce [1,2].

For that reason, in this work we present an in situ IR study (Figure 1) of the water ice formation under controlled atmosphere in presence of molecules of astrochemical interest (CO_2, NH_3, CH_3OH, etc) on the surface of an inert material (silicon wafer) and on mineral of astrochemical interest (Mg_2SiO_4, SiO_2, MgO). Finally, the results obtained from the adsorption of 2nd-period element bearing molecules (H_2S, SO_2, HCl, CH_3Cl, etc) on the bare minerals and on different ices surfaces will be exposed.

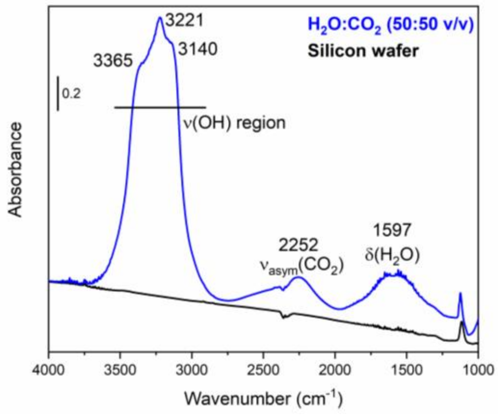


Figure 1: *IR spectra of dirty ice formed in presence of CO_2 on a silicon wafer at ~ 100 K.*

1. R.T. Garrod, E. Herbst, *Astron. Astrophys.* **2006**, 457, 927-936
2. F. Kruczkiewicz, J. Vitorino, E. Congiu, P. Theulé, F. Dulieu, *Astron. Astrophys.* **2021**, 652, A29

Diffusion and sublimation of ices on comets and (icy)moons.

Stephanie Cazaux[1,2] , Carla Tamai[1], Belen Mate[3], and Miguel Angel Satorre[4]

[1] Faculty of Aerospace Engineering, Delft University of Technology, Delft, The Netherlands
e-mail: s.m.cazaux@tudelft.nl
[2] Leiden Observatory, Leiden University, P.O. Box 9513, NL 2300 RA Leiden, The Netherlands
[3]Instituto de Estructura de la Materia, IEM-CSIC, Calle Serrano 121, 28006 Madrid, Spain
[4] Escuela Politecnica Superior de Alcoy, Universitat Politecnica de Valencia, 03801 Alicante, Spain

In this talk, the diffusion and sublimation of ice species on comets and icy moons will be discussed. Cometary ices, mainly dominated by water, formed 4.6 Gyrs ago in the solar nebula, and detain key information on the formation conditions of comets. Release of cometary ices due to sublimation is usually accompanied by the release of volatile such as CO_2, CH_4 that are present in lower abundances (Bockelée-Morvan et al. 2004). As comets approach the Sun, the release of water and volatiles increases until perihelion, and then decreases as the distance to perihelion increases (Stern et al. 1999; Biver et al. 1997b; Snodgrass et al. 2016). The desorption patterns of water and volatiles as comets approach or move away from the Sun have been reported in Biver et al. (1997a, 2002) and Rubin et al. (2020) for comets Hale Bopp and 67P/Churyumov-Gerasimenko. Experiments have been performed to study the sublimation of volatiles (CH_4) through amorphous solid water (ASW), with a focus on the structural changes in water and the influence of dust layers (as proxy for the dusty crust) during thermal processing. It appeared that the structural changes of water ice drive volatile and hyper-volatile sublimation, due to its transition from high to low intrinsic density and transformation from amorphous to crystalline. This desorption indicates that such material has been deposited at low temperatures, according to theories on cometary ices formed in the solar nebula. During the experimental temperature cycles, most of the released material is seen to be pristine.

On icy moons volatiles such as CO_2 are observed to be present on the surface (Combe et al. 2019), mixed either with water ices or non-ice material, but are known to have very short lifetimes on the surface. This indicates that these volatiles are reformed either by diffusing through kilometers of water ice as from the sub-surface ocean, as it is the case for Enceladus (Matson et al. 2008), or through redeposition of the exosphere. These volatiles, and how they diffuse and are found on the surface, could be indicators of the composition of the sub-surface oceans on icy moons.

1. Biver, N., Bockelée-Morvan, D., Colom, P., et al. 1997a, Science, 275, 1915
2. Biver, N., Bockelée-Morvan, D., Colom, P., et al. 1997b, Earth, Moon, and Planets, 78, 5
3. Biver, N., Bockel Bockelée-Morvan, D., Colom, P., et al. 2002, in Cometary Science after Hale-Bopp (Springer), 5–14
4. Bockelée-Morvan, D., Crovisier, J., Mumma, M. J., & Weaver, H. A. 2004, Comets II, 1, 391
5. Combe J.P., McCord, T., Matson, D., et al. 2019, Icarus, 317, 491-508
6. Matson, D, Davies, A.G., Johnson, T., et al. 2018, Icarus, 302, 18-26
7. Rubin, M., Engrand, C., Snodgrass, C., et al. 2020, Space science reviews, 216, 1
8. Snodgrass, C., Opitom, C., de Val-Borro, M., et al. 2016, Monthly Notices of the Royal Astronomical Society, 462, S138
9. Stern, S. A., Colwell, W. B., Festou, M. C., et al. 1999, The Astronomical Journal, 118, 1120

Laboratory constraints on thermal desorption of astrophysical ice analogues

F. Kruczkiewicz[1,2,3], F. Dulieu[2], B. M. Giuliano[3], A. V. Ivlev[3], P. Caselli[3], C. Ceccarelli[4] and P. Theulé[1]

[1] Aix Marseille Univ, CNRS, CNES, LAM, Marseille - FRANCE
[3] CY Cergy Paris Université, Observatoire de Paris, PSL University, Cergy – FRANCE
[2] Max-Planck-Institut für extraterrestrische Physik, Gießenbachstraße 1, Garching - GERMANY
[4]Université Grenoble Alpes, CNRS, IPAG, 38000 Grenoble, FRANCE
e-mail: franciele.kruczkiewicz@lam.fr

Understanding the interplay between gas accretion and gas sublimation in different astrophysical environments is crucial for comprehending the chemical evolution of the interstellar medium. Astrochemical models must accurately reflect the ratio between gas-phase and solid-phase abundances to explain grain growth/destruction in warm media, ice mantle formation/sublimation in cold media, and the resulting gas line emission spectroscopy. In star-forming regions, the mechanisms of ice sublimation play a critical role in determining the composition of the gas released and the material locked and incorporated into planetary bodies. Correctly modelling these desorption processes is essential for interpreting observations from the extra-galactic, the galactic interstellar medium and of the interplanetary medium.

In this study, we present targeted ice sublimation experiments designed to benchmark current astrochemical models. We conducted temperature-programmed desorption experiments using molecular beams in ultra-high vacuum conditions (10^{-10} hPa) and low temperatures (10 K) with increasing levels of complexity of ice analogues of various chemical compositions and thicknesses (3-80 ML), including pure ices made of Ar, CO, CO_2, NH_3, CH_3OH, H_2O, and $NH_4^+HCOO^-$, their binary ice mixtures with compact amorphous H_2O, ternary mixtures of H_2O:CH_3OH:CO, and water ice made *in situ*.

Our findings reveal common trends in the desorption of molecules compared to water: compact amorphous water ices can trap up to 20% of high volatiles, approximately 5% of H-bonded molecules, and semi-volatile species are not trapped in the water ice matrix. We conclude that deposited or formed very compact, amorphous water ice with fewer than 100 layers cannot trap a large fraction of other gases, including CO or CO2. To be reliable, astrochemical models should reproduce desorption kinetics and trapping fractions from our benchmark laboratory experiments.

Sticking Coefficients of Astrochemically-Relevant Ices on Realistic Grains Analogues are Lower than Expected

Caroline Stadler[1], Daniel Ferry[1], Olivier Grauby[1], Philippe Parent[1], and Carine Laffon[1]

[1]*Aix Marseille Univ, CNRS, CINaM, Marseille, France*

e-mail: caroline.stadler@univ-amu.fr

Around protostars, various molecular ices freeze out onto dust grains where they are processed by UV and X-ray radiation. An important turning point in this process is the catastrophic freeze-out of CO onto a pre-existing ice layer composed primarily of H_2O, driving a complex network of astrochemical reactions. While these processes have been studied in both a laboratory and through simulations, several physical properties of these systems still need to be considered in order to obtain a complete understanding of the context being monitored. One vital parameter is the sticking coefficient of these molecules, both on dust grains and on each other, which is most commonly assumed to be 1, as confirmed by previous laboratory measurements. [1]

This study provides a review of a laboratory study in which CO and N_2 ice were frozen onto carbon and olivine nanoparticle substrates, both dry and pre-emptively covered with a layer of water ice, to provide a study more relevant to an astrophysical context. Each successive layer(s) of molecules added were analyzed using both FTIR and XPS. The results of these methods were compared to the amount of gas-phase molecules injected into the system, to determine how much of each gas stuck to the substrate. It was demonstrated that the sticking coefficients of both CO and N_2 on realistic dust grain analogues are considerably lower than 1. This confirms the results previously obtained by Laffon et al [2] with H_2O and CO_2.

1. J. He, K. Acharyya, G. Vidali, *ApJ.* **2016**, 823, 56
2. C. Laffon, D. Ferry, O. Grauby, P.Parent, *Nature Astronomy.* **2021,** 5, 445-450

Unlocking the Interaction of the CN Radical with Interstellar Ices: An Atomistic View of Polar and Apolar Environments

Joan Enrique-Romero[1], Thanja Lamberts[1,2]

[1] Leiden Institute of Chemistry, Gorlaeus Laboratories, Leiden University, P.O. Box 9502, 2300 RA Leiden, THE NETHERLANDS

[2] Leiden Observatory, Leiden University, P.O. Box 9513, 2300 RA Leiden,

The Netherlands

e-mail: j.enrique.romero@lic.leidenuniv.nl

The CN radical has been observed in a variety of interstellar sources including cold molecular clouds, with an average fractional abundance (with respect to H_2) of around 10^{-10} (1,2) and has been observed in the gas phase past the CO depletion density (1,3). Given the low temperatures and increasing densities during the star formation stages, eventually CN radicals will adsorb and interact with interstellar ices (4). Depending on the exact freeze-out timescale, either H_2O- or CO-dominated ices are relevant.

CN is known to sport interactions stronger than typical H-bonding with non-classical character called hemibonds with water ices (e.g., 5). In this contribution, we present a detailed computational chemistry study on the interaction of the CN radical in both water and carbon monoxide ices. Firstly, we show an intricate benchmark including multireference effects pivotal to accurately treat adsorption. Furthermore, we discuss the capability of the CN radical to establish strong interactions with ice components and how this affects the binding energy distribution. Finally, we will show far-reaching consequences for CN reactivity, comparing polar with non-polar ices.

1. P. Hily-Blant, M. Walmsley, G. Pineau Des Forêts, & D. Flower, Astron. Astrophys., **2008**, 480(1), L5–L8.

2. A. G. G. M. Tielens, Rev. Mod. Phys., **2013**, 85(3), 1021–1081.

3. G. Pineau des Forets, E. Roueff, & D. R. Flower, Mon. Notices Royal Astron. Soc., **1990**, 244, 668–674.

4. P. Caselli, J. E. Pineda, O. Sipilä, et al., Astrophys. J., **2022**, 929(1), 13.

5. A. Rimola, D. Skouteris, N. Balucani, C. Ceccarelli, J. Enrique-Romero, V. Taquet, & P. Ugliengo, ACS Earth Space Chem., **2018**, 2(7), 720–734.

Molecular complexity in Solar-System analogs

Eleonora Bianchi[1]

[1]*Excellence Cluster ORIGINS, Boltzmannstraße 2, 85748, Garching bei München, – GERMANY*

e-mail: eleonora.bianchi@origins-cluster.de

How molecular complexity emerges and evolves during the process leading to the formation of a Sun and its planetary system?
Planets are the natural outcome of a complex process, starting in the early evolutionary stages in the protostellar disk[1] (Class 0/I stage, age $\leq 10^5$ yr). Observations of the inner protostellar regions (~ 100 au) are thus fundamental to study the initial conditions and the chemical content available for planet formation[2,3].
Astrochemistry is a powerful tool to investigate the accretion processes taking place in the planet formation region of these embedded objects, i.e. accretion streamers, shocks, jets.
In addition, a striking chemical diversity have been observed between hot corinos sources (enriched in interstellar complex organic molecules, iCOMs[4,5]) and the Warm Carbon Chain Chemistry sources[6] (WCCC, enriched of unsaturated small carbon chains). The origin of this diversity is still unclear, as well as its impact on the chemical composition of the forming planetary systems.

In this talk I will review the observational efforts carried out in the last years to chemically characterize the inner regions of Solar-System analogs. I will summarize our current understanding of the molecular complexity in young protostellar disks and the main open questions.
Finally, I will stress the importance of future radio observations (ALMA Band 1, SKA, ngVLA) to investigate the chemistry in the planet formation region.

1. ALMA Partnership et al. 201, *ApJL*, **2015**, 808, L3

2. C. Ceccarelli, C. Codella, N. Balucani, D. Bockelée-Morvan, E. Herbst, C. Vastel, P. Caselli, C. Favre, B. Lefloch, K. Öberg, S. Yamamoto, *Chapter for Protostars & Planets VII* **2022**

3. K. Öberg and E. A. Bergin, *Phys. Rep*. **2021**, 893, 1-48

4. Ceccarelli C., *Star Formation in the ISM* **2004**, vol. 323 of Astr.Soc.PacificConf. (D. Johnstone and et al.), p. 195

5. E. Herbst and E. F. van Dishoeck, *ARA&A* **2009**, 47, 427–480.

6. N. Sakai and S. Yamamoto, *Chem. Rev.* **2013**, 113, 8981-9015

A Challenging Quest to Unveil the Beyond-the-Second-Period Chemistry in Space

M. Michielan[1], D. Ascenzi[1], N. Balucani[2,3,4], G. Di Genova[2], and C. Ceccarelli[3]

[1] University of Trento, Department of Physics, 38123 Povo - ITALY;

[2] University of Perugia, Department of Chemistry, Biology and Biotechnology, 06123 Perugia – ITALY;

[3] Université Grenoble Alpes, CNRS, IPAG, 38000 Grenoble - FRANCE;

[4] Arcetri Astrophysical Observatory, 50125 Firenze – ITALY;

e-mail: matteo.michielan@unitn.it

The chemistry in space is prolific and ubiquitous despite the harsh nature of the environments involved. Understanding how molecules are formed and destroyed is paramount to giving an insight into the history, properties, and evolution of astronomical objects in which such species have been detected. The theoretical and experimental knowledge of the mechanistic aspects of these formation/destruction processes, involving neutral and ionic species, is then fundamental.

Mimicking and extending the combined chemical-astronomical approach used to investigate the chemistry of the so-called interstellar Complex Organic Molecules (iCOMs)[1,2], which interest is strongly related to the development of prebiotic molecules in space, we aim to shed light on the chemical processes involving species containing beyond-the-2nd-period elements. Many of them are indeed significantly abundant in space and some of their compounds (*e.g.*, SiO, SiS, SiP, SiN, H_2CS, CH_3SH)[3] have been already detected. With a primary interest to gain more insights into how our Solar System is formed, we focus on the reactions happening in Sun-like star-forming regions. Furthermore, understanding such chemistry would allow us to gather more information on species leading to prebiotic molecules (other than iCOMs) and/or related to the inclusion of Si into the refractory core of dust particles from which planetesimals (and then planets) are formed.

A considerable number of reactions involving such elements is listed in the available databases (*e.g.*, KIDA and UMIST), but in some cases, the information is either incomplete or incorrect (*e.g.*, unstable isomers reported as main products or rate constants lacking the temperature dependence). When available, the experimental data is often referred to past works. To critically review the aforementioned information, we herein present some preliminary results on the reactivity of different Si- and S-bearing species investigated through Guided Ion Beam Mass Spectrometer (GIB-MS) experiments.

1. P. Caselli, C. Ceccarelli, A&ARev. **2012**, 20, 56

2. E. Herbst, E.F. van Dishoeck, ARA&A. **2009**, 47, 427–480

3. http://www.astro.uni-koeln.de/cdms/molecules

Astrochemical Modeling of Protostellar Core Envelopes

Prasanta Gorai[1], Jonathan C. Tan[1,2], and Yichen Zhang[2]

[1]*Department of Space, Earth & Environment, Chalmers University of Technology, SE-412 96 Gothenburg, Sweden*
[2]*Department of Astronomy, University of Virginia, Charlottesville, VA 22904-4325, USA*

e-mail: prasanta.astro@gmail.com

A large number of molecular species have been identified in hot molecular cores, i.e., the gas that is directly involved in star formation. Chemical evolution is expected to be closely coupled to physical evolution. In particular, it is crucial to include the evolution of densities and temperatures along infalling streamlines in the chemical modeling to predict the spatial distribution of abundances in protostellar core envelopes. Here we present an astrochemical model of protostellar core envelopes based on the framework of the Turbulent Core Accretion model (McKee & Tan 2003; Zhang et al. 2014). We discuss the evolution of abundances in the ice and gas phases within a 60 solar mass core that eventually forms a 1, 4, 8, 12, 16, 20, and 24 solar mass star. The location of ice lines in the infall envelope is one particular focus. We compare the results of these models to observed properties of hot cores.

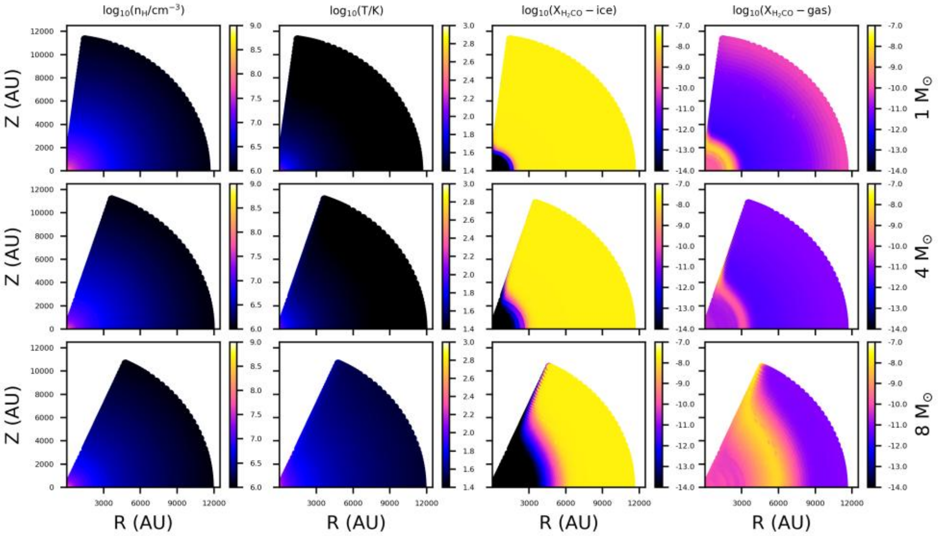


Figure 1: *Example of theoretical modeling, showing a slice of the astrochemical structure of density (first column), temperature (second column), and H_2CO ice phase abundance (third column) and gas phase abundance (fourth column) of the infalling envelope around $m_* = 1, 4, 8 M_\odot$ protostars (top to bottom rows, respectively) forming from an initially 60 $M_\odot$ core (protostar is in the lower left corner, Gorai et al. in prep.)*

1. P. Gorai, J. C. Tan, Y. Zhang, **2023**, in prep
2. Y. Zhang, J. C. Tan, T. Hosokawa, ApJ, **2014**, 788, 166
3. C. F. McKee, J. C. Tan, ApJ, **2003**, 585, 850

Comparing the Reactivity of HCN and $HCONH_2$ on Amorphous and Crystalline Mg_2SiO_4 Surfaces: Insights into Interstellar Dust Grain Chemistry

Rosangela Santalucia[1] , Erika Varesi[1], Guillermo Escolano Casado[1], Gloria Berlier[1], Giuseppe Spoto[1], Lorenzo Mino[1], Piero Ugliengo[1]

[1]*University of Torino, Department of Chemistry, Via Giuria 7, Torino – ITALY*

e-mail: rosangela.santalucia@unito.it

Hydrogen cyanide (HCN) and formamide ($HCONH_2$, hereafter referred to as FA) are widely recognized as crucial molecules in astro- and prebiotic chemistry, as they are involved in the formation of many of the building blocks of life, such as amino acids and nucleobases.[1,2] The abundant occurrence of HCN and FA in various astrophysical environments, including comets and interstellar regions, has prompted research to investigate their chemistry under plausible extraterrestrial conditions. Additionally, the detection of complex organic molecules (iCOMs) in the star forming regions suggests that the formation of biomolecules might have already taken place in the early stages of Solar System formation. Mineral surfaces within interstellar dust grains and comets may have acted as catalysts in the complexification of iCOMs. The majority of literature on the chemistry of the two key precursors, HCN and FA, is based on experiments performed in condensed phase and/or under harsh energetic conditions, such as temperatures exceeding 300 K or under UV/proton irradiation. However, a comprehensive study of the reactivity of HCN and FA in heterogeneous conditions, specifically at the gas phase/solid interface, is currently lacking in the literature.

To contribute to fill this gap in this study we show a comparison between the adsorption and reactivity of HCN[3] and FA at the surfaces of two Mg-silicates in amorphous (AMS) and crystalline (forsterite) form, being the major constituents of the dust grain cores in the interstellar medium and in protoplanetary disks, as well as in comets, meteorites, and asteroids. The adsorption of HCN and FA from the gas phase and their reactivity were studied by *in situ* FT-IR at 300 K. In order to evaluate the role of surface sites of such Mg-silicates in HCN/FA reactivity, we have also investigated the behaviour at the surface of two simple oxides, SiO_2 and MgO, which represent suitable model systems for the major structural building blocks of Mg_2SiO_4 samples. Despite the chemistry of HCN is closely relate to those of FA (as it is the HCN hydration product), the comparison between the two molecules has shown that only HCN in presence of Mg-silicate surfaces is able to react leading to the formation of more complex compounds including some of biological interest, such as adenine nucleobase.

1. M. Ruiz-Bermejo, M. P. Zorzano, S. Osuna-Esteban, *Life* **2013**, 3 (3), 421-48.
2. R. Saladino, C. Crestini, S. Pino, G. Costanzo, E. Di Mauro, *Phys. Life Rev.* **2012**, 9 (1), 84-104
3. R. Santalucia, M. Pazzi, F. Bonino, M. Signorile, D. Scarano, P. Ugliengo, G. Spoto, L. Mino, *Phys. Chem. Chem. Phys.* **2022**, 24 (12), 7224-7230.

Chemical Evolution During the Formation of a FHSC: the B1b-N Case

David Navarro-Almaida[1], Patrick Hennebelle[1], Benoît Commerçon[2], Maryvonne Gerin[3], Ugo Lebreuilly[1], and Asunción Fuente[4]

[1]*Departement d'Astrophysique, CEA Paris-Saclay, 91191 Gif-sur-Yvette – FRANCE*

[2]*Centre de Recherche Astrophysique de Lyon, ENS de Lyon, Lyon – FRANCE*

[3]*LERMA, Observatoire de Paris, CNRS, Sorbonne Université, Paris – FRANCE*

[4]*Observatorio Astronómico Nacional (OAN-IGN-CNIG), Madrid - SPAIN*

e-mail: david.navarroalmaida@cea.fr

In the theory of star formation, the first hydrostatic core (FHSC) phase is a critical step in which a condensed object emerges from a prestellar core, with the formation of compact circumstellar disk and wide-angle bipolar outflow. This is, however, an elusive stage due to its embedded and brief nature. On the theoretical side, non-ideal MHD simulations are state-of-the-art tools to better understanding the FHSC phase in a realistic manner. On the observational side, only high spatial resolution (~10 au) continuum and spectroscopic data can unveil the intimate structure of these objects. The comparison of numerical simulations and high spatial resolution spectroscopic data requires of an accurate description of the chemical structure of these complex and compacts objects. To determine the chemical composition of the compact circumstellar disks formed around these objects is also key to constrain their chemical properties that will be inherited to the subsequent stages of the star formation process, including protoplanetary disks and planets.

We present the products of a non-ideal MHD RAMSES simulation of a 1 $M_\odot$, strongly magnetized (μ=2) Barnard1b-like protostar reaching the FHSC phase in 65 kyr. Among the many approaches that can be followed to determine the chemical evolution and final composition of the FHSC, we used 200000 tracer particles to probe the physical properties of the collapsing core. Each particle describes a density-temperature trajectory that was postprocessed using the state-of-the-art gas-grain chemical code Nautilus and an up-to-date chemical network to obtain the chemical makeup of the FHSC and the evolution of the chemical abundances through time. A detailed analysis of the chemical composition of the compact circumstellar disk and the surrounding warm and flattened envelope is done. Our results indicate that adsorption, grain-phase reactions, and thermal desorption are the main drivers of the chemical evolution from the prestellar to the FHSC stage. We detected a lack of gas-phase CO in the compact disk formed in the FHSC phase as a consequence of the enhancement of organic molecules like H_2CO or CH_3OH. This chemical processing is a direct consequence of the physical evolution of the protostar, and it is not reproduced with simple two-phase chemical models. Finally, we examined the effects of grain size in the chemistry of the FHSC allowing dust growth in the density-temperature trajectories sampled by tracer particles present in the simulation.

Chemical Environment Of Emerging Hot Cores: The Early Warm-Up Phase Chemistry

Laure Bouscasse[1] and Timea Csengeri[2]

[1]*IRAM, 300 rue de la Piscine 38400 Saint Martin d'Hères- FRANCE*

[2] Laboratoire d'Astrophysique de Bordeaux, Univ. Bordeaux, CNRS, B18N, allée Geoffroy Saint-Hilaire, 33615 Pessac - FRANCE

e-mail: bouscasse@iram.fr

The physical processes at the origin of high-mass stars are still poorly constrained. ALMA has been extremely successful to identify a large sample of high-mass protostars in early evolutionary stages (high-mass equivalents of Class 0 protostars) in the frame of the SPARKS survey.

From these, six sources have been found to be isolated down to 400au, which were selected to study the early warm-up phase chemistry leading to the emergence of hot cores. These sources have been studied using an unbiased spectral survey between 159 and 374 GHz with the APEX telescope and revealed a rich molecular emission even towards the youngest sources. Although the sources have a common molecular reservoir composed of the simplest molecules, we detect COMs in the cold component of the envelope for all objects. We find that one of the main differences in the molecular emission of our sources is for the COMs. We pinpoint a gradual emergence of the warm component and an increasing molecular complexity along the evolutionary sequence of the targets. The comparison of the molecular composition of our objects to that of a sample of hot cores and hot corinos suggests strong similarities for O-bearing COMs. Overall, we propose a new evolutionary stage prior to the emergence of hot cores, where molecular abundances of COMs are lower than that of hot cores and resemble more that of hot corinos (Bouscasse et al. 2022, subm).

We extended our study to carbon chain molecules in the cold envelope of high-mass clumps with the 3mm band of the IRAM-30m revealing that high-mass star forming regions are also rich in carbon chain molecules. They exhibit strong similarities to WCCC objects (Bouscasse et al. in prep.). These new results are challenging our current view on the dichotomy between WCCC and hot corino chemistries.

1. Bouscasse et al. 2022, A&A, 662, A32
2. Bouscasse et al. subm, 2023

Solid Interstellar Radical Chemistry (SIRC): A New Methodology to Study Radical Reactivity in Interstellar Ice Analogues

F. Duvernay[1], A. Gutiérrez-Quintanilla[1], Y. Layssac[1], T. Butscher[1], S. Henkel[2], Y.A. Tsegaw[2], D. Grote[2], W. Sander[2], and T. Chiavassa[1]

[1]Aix Marseille Univ, CNRS, PIIM, Marseille, France

[2]Lehrstuhl für Organische Chemie II, Ruhr-Universität Bochum, 44780 Bochum, Germany

e-mail: fabrice.duvernay@univ-amu.fr

The interstellar medium (ISM) is composed of 99 % gas and 1 % dust, by mass. In dense molecular clouds, where matter is concentrated, the temperature is about 10 K, leading to the condensation of atoms and molecules on solid grains forming interstellar ices. Among the molecules that compose these ices, we find water (H_2O), carbon monoxide (CO), formaldehyde (H_2CO), and methanol (CH_3OH). These molecules are constantly bombarded by energetic photons (UV, X) and particles (H^+, e^-, heavy ions) coming from the surrounding stars. The energy input is sufficient to break chemical bonds and then form radical species whose reactivity can lead to more complex molecules[1,2]. The study of the formation of these molecules is of special interest because interstellar ices represent an efficient chemical reactor and the products are incorporated in the asteroids, comets, and planets of forming stellar systems.

To better understand the chemistry of the ISM, we have simulated these processes in the laboratory using a physical chemistry experiment, that allows the generation of ice analogs on a cold finger (11 K) and under vacuum conditions (10^{-9} mbar). We use a hydrogen plasma lamp to mimic the UV radiation (Lyman-α :121.6 nm/10.2 eV) of a nearby star and initiate free radical reactivity processes within the sample. Nevertheless, the radical intermediates formed in the interstellar ice analogues are difficult to detect by classical analytical techniques such as infrared spectroscopy or mass spectrometry. It is therefore impossible to conclude on the reaction pathways taking place in our samples.[3] This is why the central objective of this project is to develop new methodologies allowing the characterization of radicals as well as the control of radical reactivity in ice analogs. Our main results show that the use of cryogenic noble gas matrix isolation technique and electron paramagnetic resonance spectroscopy for sample analysis are extremely promising tools to draw accurate reaction schemes. With the use of this new methodology, about ten radicals and many relevant products for ISM chemistry such as glycolaldehyde, methyl formate, sugars, and carboxylic acid have been characterized allowing to better constraint formation mechanisms[3,4].

1.K.-J. Chuang, G. Fedoseev, D. Qasim, S. Ioppolo, E. van Dishoeck, H. Linnartz, *MNRAS*. **2017**, 467, 2552

2.C. J. Bennett, R.I. Kaiser, *ApJ*. **2007**, 661, 899

3.A. Gutiérez-Quintanilla, Y. Layssac, T. Butscher et al., *MNRAS*. **2021**, 506, 3734-3750

4.Y. Layssac, A. Gutiérez-Quintanilla, T. Chiavassa, F. Duvernay, *MNRAS*. **2020**, 496, 5292-5307

Computational Approach for the High-Throughput Screening of Molecular Interactions for Prebiotic Astrocatalysis

Eric Mates-Torres[1], Albert Rimola[1]

[1] *QuantumGrain, Departament de Química, Universitat Autònoma de Barcelona, 08193 Bellaterra, Catalonia*

e-mail: eric.mates@uab.cat

Interstellar grains and cometary and meteoritic seeds have undoubtedly been found to be key for the formation of interstellar simple and complex organic molecules (iCOMs).[1] To this date, 241 molecular species have been identified in our galaxy and beyond.[2] Many works have focused on identifying the effect that the interstellar bodies play on the formation process of these molecules; however, computational studies have mainly focused on the role of the icy surfaces that usually surround them, for at initial stages of planetary formation, these have been shown to provide surface sites where primordial molecules adsorb, diffuse and eventually react.

In our study, the vast diversity of materials present in the currently analysed stellar objects and the predicted presence of liquid water and exposed mineral surfaces in the latter stages of planetary evolution[3] led us to assess how the solid surface of interstellar, cometary and meteoritic grains interact with the molecular species in the interstellar medium. While the former are usually composed of silicates and pyroxenes of different compositions, *ca.* 275 different minerals have been found to constitute the latter two.[4] In order to thoroughly study this variety of surface compositions and interacting molecular species, we propose a novel and unexplored approach to automatically investigate, using state-of-the-art quantum chemistry simulations, how molecules in the observed universe interact with the known mineral surfaces of most common interstellar bodies. This thorough analysis will lay down the path to rationalise astronomical observations, as well as provide a foundation for the investigation of how prebiotic molecular species, such as amino acids and sugars, are formed at the latter stages of planetary formation.

1. Molpeceres, G.; Rimola, A.; Ceccarelli, C.; Kästner, J.; Ugliengo, P.; Maté, B. *MNRAS* **2019**, 482, 5389–5400.
2. McGuire, B. A., *Astrophys. J., Suppl. Ser.* **2022**, 259, 51.
3. Muneishi, K.; Naraoka, H., *Meteorit. Planet. Sci.* **2021**, 56, 195–205.
4. Rubin, A. E., *Meteorit. Planet. Sci.* **1997**, 32, 231–247.

Constraining the Diffuse Envelope Surrounding L1544

J. Ferrer Asensio[1], S. Spezzano[1], P. Caselli[1], S. Jensen[1], O. Sipilä[1], E. Redaelli[1], F. Alves[1]

[1]*Center for Astrochemical Studies, Max-Planck-Institute for Extraterrestrial Physics,*
Gießenbachstraße 1, Garching bei München, GERMANY
e-mail: ferrer@mpe.mpg,de

Prestellar cores are gravitationally contracting fragments of molecular clouds, on the verge of star formation[1]. Their chemical richness allows for a detailed analysis of their physical properties via molecular spectroscopy. Observations towards the dust peak of the prestellar core L1544 have shown multiple molecular tracers that present a double-peaked line profile[234567]. The possible reasons behind this line morphology encompass self-absorption, the presence of two velocity components on the line of sight, depletion towards the core centre and radiative transfer in a contracting centrally concentrated dense core[2367]. To investigate these scenarios and constrain the chemical structure of the core and the surrounding envelope, we derive abundance profiles from high-sensitivity and high-spectral resolution observations of molecular species and their ^{13}C and ^{34}S -bearing isotopologues known to trace both the core and the envelope: HCO^+, CS, SO, H_2CO and c-C_3H_2[8]. We reproduce the observations with gas-grain chemical simulations[9] applied to a physical model of L1544 presented by Keto & Caselli[10] and using non-LTE radiative transfer modelling coupled with the Monte Carlo method. The abundance profile (defined as step function), the turbulence, and the scaling factor for the velocity profiles of the Keto Caselli model are used as free parameters in the radiative transfer simulation. I will present the results of this approach, where we can fully exploit molecular line emission as an astrophysical tool, and study the connection between the core and its surrounding envelope for the prototypical prestellar core L1544.

[1] André et al. 2000
[2] Tafalla et al. 1998
[3] Williams et al. 1999
[4] Dore et al. 2001
[5] Tafalla et al. 2002
[6] Caselli et al. 2002
[7] Ferrer Asensio et al. 2022
[8] Ferrer Asensio et al. 2023 (in prep.)
[9] Sipilä et al. 2015
[10] Keto et al. 2015

Grain growth in star formation

Pierre Marchand[1]

[1]*Institut de Recherche en Astrophysique et Planétologie, 9 avenue du Colonel Roche, 31400 Toulouse*

e-mail: pierre.marchand@irap.omp.eu

Grains play a major role in all astrophysical processes: radiative transfer, chemistry, ionization, planet formation... Although their size is badly constrained, we know that they grow by coagulation during star formation. However, their physics adds a lot of complexity, therefore they have rarely been included in numerical calculations. Using a fast calculation method that I have recently developed, I will present 3D non-ideal MagnetoHydroDynamics simulations of protostellar collapses including grain growth, as well as analytical models that can be used for astro-chemical modeling.

1. P. Marchand, V. Guillet, U. Lebreuilly, M.-M. Mac Low, *A&A*. **2021**, 649, A50
2. P. Marchand, U. Lebreuilly, M.-M. Mac Low, V. Guillet, *A&A*. **2023**, 670, 61

Ion-neutral reactions for formation and destruction of interstellar Complex Organic Molecules

Daniela Ascenzi[1], Christian Alcaraz[2,3], Claire Romanzin[2,3], Roland Thissen[2,3], Vincent Richardson[1,4], David Sundelin[5], Wolf Geppert[5], Miroslav Polášek[6], Emília Valença Ferreira de Aragão[7], Noelia Faginas-Lago[7], Marzio Rosi[7] and Fernando Pirani[7]

[1]*University of Trento, Department of Physics, Via Sommarive 14, Trento –ITALY*
[2] *Institut de Chimie Physique, Université Paris-Saclay, CNRS, Orsay - FRANCE*
[3] *Synchrotron Soleil, Saint Aubin - FRANCE*
[4] *University of Liverpool, Department of Physics, Oxford St, Liverpool – UK*
[5] *Department of Physics, Stockholm University, Stockholm – SWEDEN*
[6] *J. Heyrovsky Institute of Physical Chemistry, AVCR, Prague – CZECH REPUBLIC*
[7] *Department of Chemistry, Biology and Biotechnology, University of Perugia, Perugia - ITALY*
e-mail: daniela.ascenzi@unitn.it

Interstellar complex organic molecules (iCOMs) have been detected at various phases of stellar evolution, from the pre-stellar cloud stage to the protostar and protoplanetary disk phase, and they represent important tracers of the physical conditions of the astrophysical object in which they are detected. While being less abundant, and hence more difficult to detect with respect to neutrals, molecular ions can play a key role either in the formation or in the decomposition of iCOMs. In the former case, the usually fast and barrierless ion-molecule reactions can lead to the synthesis of larger ionic species, which, upon subsequent neutralization processes (e.g. by dissociative recombination with electrons or proton transfers), can generate more complex neutrals. In the latter case, collisions between organic molecules and highly energetic ions (e.g. He^+) will result in the capture of an electron from an inner valence orbital of the organic molecule, leaving the latter in highly excited electronic states, thus leading to molecular fragmentation. In this contribution we will review recent results on the laboratory measurements of kinetic parameters (cross sections, branching ratios and their dependences on collision energy) for the reaction of charged molecules with neutrals, by using tandem mass spectrometric techniques and RF octupolar trapping of parent and product ions. Experimental results are complemented by theoretical calculations of the most relevant stationary points on the potential energy (hyper)surfaces in support of reaction mechanisms and to estimate rate constants.

As an example of the first type of ion-molecule processes (synthesis of larger ionic species) we will present the reactivity of the two radical cation isomers methanimine ($H_2CNH^{+\cdot}$) and aminomethylene ($HCNH_2^{+\cdot}$) with saturated and unsaturated hydrocarbons, nitriles and O-containing species [1-3]. Results indicate that reactions do lead to molecular growth, with isomer-dependent reaction mechanisms and product yields. As an example of the second type of processes (destruction of molecular complexity) we will present the reactions of He^+ with O- and N- containing iCOMs (CH_3OH [4] and CH_3CN). In this case the main result is that charge exchange processes are completely dissociative, but the observed branching ratios and cross sections can be quite different from those predicted by simple capture models.

1. V. Richardson, C. Alcaraz, et al. *Chem. Phys. Lett.* **2021,** 775, 138611.
2. D. Sundelin, D. Ascenzi, et al. *Chem. Phys. Lett.* **2021**, 777, 138677.
3. V. Richardson, D. Ascenzi, et al. *Front. Astron. Space Sci.* **2021**, 8, 752376.
4. V. Richardson, E. V. F. de Aragão et al. *PCCP* **2022**, 24, 22437.

Gas-Phase Formation Of Interstellar Methyl Cyanide: Review And New Theoretical Calculations

L.Giani[1] , C.Ceccarelli[1], L.Mancini[2], E.Bianchi[3], M. Rosi[4], F.Pirani[4,5] and N.Balucani[2]

[1]*Univ. Grenoble Alpes, CNRS, IPAG, 38000 Grenoble, France*

[2]*Dipartimento di Chimica, Biologia e Biotecnologie, Università degli Studi di Perugia, Perugia, 06123, Italy*

[3]*Excellence Cluster ORIGINS, Boltzmannstraße 2, 85748 Garching bei München, Germany*

[4]*Dipartimento di Ingegneria Civile e Ambientale, Università degli Studi di Perugia, Perugia, 06125, Italy*

[5]*Master-Tec s.r.l., Via Sicilia 41, Perugia, 06128, Italy*

e-mail: lisa.giani@univ-grenoble-alpes.fr

Recent studies suggest that nitrile-bearing molecules, characterized by the C≡N functionality, played a crucial role in prebiotic chemistry in the syntheses of RNA and protein precursors[1,2]. Methyl cyanide (CH_3CN) is one of the most abundant interstellar complex organic molecules and widely detected, but its formation is still debated.

In this work, we present a new gas-phase chemical network, whose scheme is shown in Fig. 1. We reviewed the products and kinetic rates of each reaction and we included new paths. Some reactions, marked red in the figure, included in the databases KIDA and UMIST, resulted to have wrong data and were removed. Other reactions, shown in blue in the figure, were not studied via laboratory or theoretical works. In these cases, we carried out new quantum mechanical (QM) calculations followed by a theoretical kinetic analysis (using a semiempirical entrance potential and RRKM theory) to obtain accurate values of the rate constants at low temperatures (10-300 K). Finally, we coupled our new computations with a chemical modeling analysis to check the relative importance of all the reactions in the network, depending on the physical conditions.

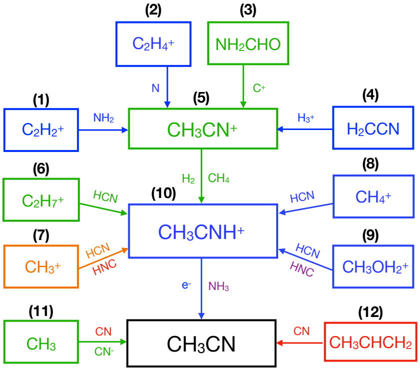


Figure 1: *Scheme of the gas-phase formation routes of methyl cyanide proposed in the literature. The blue boxes mark the reactions studied in the present work of which the plum ones are newly proposed. The red boxes mark the reactions which we suggest to remove from the network. The orange box marks a reaction that is used with an updated rate coefficient derived from the literature, while the green ones are the verified reactions.*

1. M. W. Powner, B. Gerland, and J. D. Sutherland, *Nature,* **459** 239–42 (2009)
2. J. D. Sutherland, *Angew. Chem. Int. Ed.*, **55** 104-121 (2016)

Formation and elongation of polyglycine via unimolecular reaction in the gas phase

P. Bertier[1], H. Lissillour[1], L. Parrado Ospina[1], D. Comte[1,4], L. Lavy[1], P. Calabria[1], R. Fillol[1], F. Calvo[2], I. Daniel[3], B. Farizon[1], M. Farizon[1], T. D. Märk[4]

[1] Université Lyon 1, CNRS/IN2P3, UMR 5822, Institut de Physique des 2 Infinis de Lyon, F 69622 Villeurbanne, FRANCE

[2] Université Grenoble Alpes, CNRS LIPHY-38000 Grenoble, FRANCE

[3] Université Lyon 1, Ens Lyon, CNRS, UMR 5276, LGL-TPE, F 69342, Lyon, FRANCE

[4] Institut für Ionenphysik und Angewandte Physik, Leopold Franzens Universität 6020 Innsbruck, AUSTRIA

e-mail: p.bertier@ip2i.in2p3.fr

Peptide chains of amino acids play a crucial role in the emergence of living organisms. Understanding the growth of peptide chains under abiotic conditions is an important question, especially considering the increasing amount of complex molecules detected in various astrophysical environments [1]. Gas-phase collisions between isolated molecules or cosmic ray-induced reactions in seeded ice and dust grains are presently the main pathways considered for polymer synthesis under astrophysical conditions. Recently, we found that the growth of peptide chains can occur under gas-phase conditions via a dehydration reaction in a protonated molecular amino acid dimer ion [2]. Combining experimental results and quantum chemistry calculations, we show that polymerization reaction leading to the peptide of glycine (diglycine) is taking place after excitation of a protonated glycine dimer in a single high velocity collision, and we provide evidence the further growth of the peptide chain. The formation of a protonated mixed dimer consisting of a diglycine and a glycine molecule is dominant and its further excitation can lead to the formation of a tripeptide. The various relaxation pathways of the excited protonated dimers and the unimolecular reaction dynamics is investigated by velocity measurements of the water molecules eliminated in the polymerization reactions. The proton facilitates the dehydration reaction in a pure molecular dimer and chaperons the further growth of the peptide-chain via further dehydration reactions in mixed dimer and cluster ions. These results obtained with glycine, the most abundant amino acid detected in extraterrestrial objects, shows that the detected intra-dimer dehydration reaction could be a conceivable abiotic pathway towards the possible existence of peptide chains in Space.

1 – Pearce, B.; Pudritz, R. E.; Semenov, D. A.; Henning, T. K. Proc. Natl. Acad. Sci. U.S.A. **2017**, 114, 11327–11332.

2 – D. Comte, L. Lavy, P. Bertier, F. Calvo, I. Daniel, B. Farizon, M. Farizon, T. D. J. Phys. Chem. A **2023**, 127, 3, 775–780.

OMC-2 FIR4: a protostellar cluster full of surprises.

L. Chahine[1], A. Lòpez-Sepulcre[1], R. Neri[2], S. Mercimek[3], L. Podio[3], C. Codella[3,1], C. Ceccarelli[1], P. Caselli[4] and M. De Simone[5]

[1] *Univ. Grenoble Alpes, CNRS, IPAG, 38000 Grenoble, France*
[2] *Institut de Radioastronomie Millimétrique (IRAM), 38406 Saint-Martin-d'Hères, France*
[3] *INAF, Osservatorio Astrofisico di Arcetri, Largo E. Fermi 5, I-50125, Firenze, Italy*
[4] *Center for Astrochemical Studies, Max Planck Institute for Extraterrestrial Physics, 85748 Garching, Germany*
[6] *ESO, European Southern Observatory, 85748 Garching, Germany*
e-mail: layal.chahine@univ-grenoble-alpes.fr

Our Sun was born in a densely packed star cluster, near massive stars[1] whose energetic radiation must have contributed to shaping the evolution of the surrounding environment. How does all of this affect the physics and chemistry of the proto-Sun-like objects and their immediate surroundings is still an open question.

A perfect target to answer this question is the protostellar cluster OMC-2 FIR4. It is located along the Orion Integral Shape Filament, ~2 pc north of the Trapezium OB stellar cluster and ~0.04 pc south of the protostar HOPS-370, noted for its high velocity outflow[2]. OMC-2 FIR4 is considered as the nearest analogue of the environment in which the Sun may have been born. In this context, we used ALMA observations at 1.3mm to investigate how this protocluster appears at small (~100-800 au) scales in multiple molecular tracers. We carried out a detailed chemical study on the sun-like protostar HOPS-108, and we detected 11 interstellar Complex Organic Molecules (iCOMs). This hot corino showed an enhancement of the $HCOOCH_3$ abundance and a low $[CH_2DOH]/[CH_3OH]$ ratio (~2.5%) compared to other hot corinos[3] indicating a possible impact from the environmental conditions. In addition, we found that HOPS-108 lies along one of the several interwoven filaments present in FIR4. This led us to characterise the immediate environment (within ~8000 au) of formation of this hot corino. We analysed the spatial distribution of dust and 8 different molecular tracers probing extended high-density structures and shocks. Our observations show that OMC-2 FIR4 consists of an intricate network of filaments with different velocities and bow shocks, attesting to the dynamical and chemical complexity[4]. We also reveal, for the first time, the presence of an elongated (~5200 au) and highly collimated wiggling SiO jet, driven by the embedded protostar VLA 15. The filaments observed at small scales in our study are likely connected to those observed at ~1 pc scales[5]. However, their kinematics might be altered by internal and/or external mechanisms such as protostellar feedback. These filaments appear to be connected to the protostars and thus may provide preferential routes of material accretion onto the future stellar systems.

References:

1. Adams, F. C. 2010, ARA&A, 48, 47
2. Shimajiri, Y., Takahashi, S., Takakuwa, S., Saito, M., & Kawabe, R. 2008, ApJ, 683, 255
3. Chahine, L., Lòpez-Sepulcre, A., Neri, R., et al. 2022, A&A, 657, A78
4. Chahine, L., Lòpez-Sepulcre, A., Podio, L. et al 2022, A&A, 667, A6
5. Hacar, A., Tafalla, M., Forbrich, J., et al. 2018, A&A, 610, A77

Molecular fractionation from clouds to planetary systems

Eva Wirström[1]

[1] *Chalmers University of Technology, Department of Space, Earth and Environment, Onsala Space Observatory, SE-439 92 Onsala – SWEDEN*

e-mail: eva.wirstrom@chalmers.se

Isotope ratios of foremost hydrogen, carbon and nitrogen in molecules are considered important tools in tracing the chemical heritage of material through the process of solar-type star formation, from molecular clouds to planetary systems. However, in order to apply this tool the processes that govern the distribution of isotopes between different molecular reservoirs, the fractionation processes, have to be well enough understood under a wide range of conditions. In this talk I will review the current theory of molecular fractionation based on observations and astrochemistry models as well as highlight some major challenges still ahead.

First ALMA Maps of Cosmic-Rays Ionization Rate in High-mass Star-forming Regions

Giovanni Sabatini[1] , Stefano Bovino[2] & Elena Redaelli[3]

[1]*INAF – Osservatorio Astrofisico di Arcetri, Largo E. Fermi 5, I-50125 Firenze, Italy*
[2]*Univ. de Concepción, Dept. de Astronomía, Av. E. Iturra s/n Barrio Univ., 160, Concepción, Chile*

[3]*Max-Planck-Institut für extraterrestrische Physik, Gießenbachstraße 1, D-85749 Garching bei München, Germany*

e-mail: giovanni.sabatini4@unibo.it

Low-energy cosmic rays (<1 TeV) are a pivotal source of ionisation of the interstellar medium, where they play a central role in determining the chemical gas composition and, in turn, in influencing the formation of stars and planets. Observations of H_3^+ absorption lines in diffuse clouds - $n(H_2) \sim 10^2$ cm^{-3} - have been used for decades to provide reliable estimates of the cosmic ray ionisation rate relative to molecular hydrogen (ζ_{H2}). However, in denser clouds where stars and planets form, this method is often inefficient since H_3^+, similar to H_2, does not emit rotational lines as it does not have a permanent electric dipole. The ζ_{H2} estimates are therefore still provisional in this context, and represent one of the least understood ingredient when it comes to defining general models of star formation. Recently, a new analytical approach to estimate ζ_{H2} in the densest regions of molecular clouds has been proposed by Bovino et al. (2020), based on observations of ortho-H_2D^+ as the main observational constraint to derive the amount of H_3^+. This has been applied by Sabatini et al. (2020) in a large sample of high-mass star-forming regions. Exploiting the exceptional observational capabilities of ALMA, in this talk I will present the first high-resolution maps of ζ_{H2} in two massive clumps. I will present these results and the way they provide crucial constraints for chemical/physical modelling of star-forming regions.

References

[1] Sabatini, G., Bovino, S., Giannetti, A., et al. **2020**, A&A, 644, A34
[2] Bovino, S., Ferrada-Chamorro, S., Lupi, A., et al. **2020**, MNRAS-letter, 495, L7

A high HDO/H_2O ratio in the Class I protostar L1551 IRS5

A. Andreu[1] , A. Coutens[1], F. Cruz-Sáenz de Miera[2, 3], N. Houry[1], J. K. Jørgensen[4], A. Kóspál[2, 3, 5, 6] and D. Harsono[7]

[1]*Institut de Recherche en Astrophysique et Planétologie (IRAP), Université de Toulouse, UT3-PS, CNRS, CNES, 9 av. du Colonel Roche, 31028 Toulouse Cedex 4, France*
[2] *Konkoly Observatory, Research Centre for Astronomy and Earth Sciences, Eötvös Loránd Research Network (ELKH), Konkoly-Thege Miklós út 15-17, 1121 Budapest, Hungary*
[3] *CSFK, MTA Centre of Excellence, Budapest, Konkoly Thege Miklós út 15-17, H-1121, Hungary*
[4] *Centre for Star and Planet Formation, Natural History Museum of Denmark, University of Copenhagen, Øster Voldgade 5-7, DK-1350 Copenhagen K, Denmark*
[5] *Max-Planck-Institut für Astronomie, Königstuhl 17, D-69117 Heidelberg, Germany*
[6] *Eötvös Loránd University, Department of Astronomy, Pázmány Péter sétány 1/A, 1117 Budapest, Hungary*
[7] *Institute of Astronomy, Department of Physics, National Tsing Hua University, Hsinchu, Taiwan*

e-mail: audrey.andreu@irap.omp.eu

Water molecules play a key role in the interstellar medium as they cool down the warm regions and boost the gravitational collapse leading to star formation[1]. They are also fundamental to the emergence of life. They have been detected at different stages of the star formation process from cold prestellar cores to protoplanetary disks[2]. The deuteration of water, through the HDO/H_2O and D_2O/HDO ratios, is a chemical tool used to characterize the formation of water and its evolution from the early stages of the star formation process up to its delivery to planets[3, 4]. Since then, most of the studies focused on Class 0 sources[5]. Studies on more evolved sources are needed to reconstruct the chemical evolution of water.

We will present here results regarding the water deuteration of L15551 IRS5, a Class I solar-type protostar and FUor-like object observed with the NOEMA interferometer. Thanks to these interferometric data, the water deuteration can be investigated in the innermost regions of the protostar at scales of about a 200 au which is similar to the sizes of disks in which planets form. The results will be compared to previous studies on protostars and comets.

1. C. Ceccarelli et al., *Protostars and Planets VI.* **2014**, 859-882
2. E. F. van Dishoeck et al., *A&A* **2021**, 648, A24
3. E. F. van Dishoeck, E. Herbst, D. A. Neufeld, *Chemical Reviews* **2013**, 113, 12
4. K. Furuya et al., *A&A* **2017**, 599, A40
5. S. S. Jensen et al., *A&A* **2019**, 631, A25

Formaldehyde In The Dynamic Protobinary System [BHB2007] 11: Deuteration and Streamer Kinematics

Lucy Evans[1] , Charlotte Vastel[2], Francesco Fontani[3], Jaime Pineda[4], Izaskun Jimènez-Serra[5], Mathilde Bouvier[6], Cecilia Ceccarelli[7] and the FAUST team

[1]School of Physics and Astronomy, University of Leeds, Leeds LS2 9JT - UK

[2] *IRAP, Université de Toulouse, CNRS, CNES, UPS, Toulouse - FRANCE*

[3]*INAF-Osservatorio Astrofisico di Arcetri, Largo E. Fermi 5, I-50125, Florence - ITALY*

[4]*Max-Planck-Institut für extraterrestrische Physik (MPE), Gießenbachstr. 1, D-85741 Garching - GERMANY*

[5]*Centro de Astrobiologia (CSIC-INTA), Ctra. de Torrejon a Ajalvir, km 4, 28850, Torrejon de Ardoz - SPAIN*

[6]*Leiden Observatory, Leiden University, PO Box 9513, 2300 RA Leiden - THE NETHERLANDS*

[7]*Université Grenoble Alpes, CNRS, Institut de Planètologie et d'Astrophysique de Grenoble (IPAG), 38000 Grenoble - FRANCE*

e-mail: l.e.evans@leeds.ac.uk

Deuterium in H-bearing species is enhanced during the early stages of star formation, however, only a small number of high spatial resolution deuteration studies exist towards protostellar objects, leaving an unclear picture of the small-scale structures. We observed the Class 0/I protobinary system [BHB2007] 11 using the Atacama Large Millimeter Array (ALMA) within the context of the Large Program Fifty AU STudy of the chemistry in the disk/envelope system of Solar-like protostars (FAUST). These high angular resolution observations probe the structures of the protobinary system, enabling us to resolve multiple velocity components associated with the methanol hot spots also uncovered by FAUST data (1), as well as the colder external envelope. Using radiative transfer, we constrain the column density values of detected H2CO 3(0,3)-2(0,2), HDCO 4(2,2)-3(2,1), HDCO 4(1,4)-3(1,3) and D2CO 4(0,4)-3(0,3) lines, leading to a measurement of the deuteration ratio for the first time in this source.

Furthermore, complex protostellar systems such as [BHB2007] 11 are expected to have complex kinematics even at very small angular scales; this has indeed been shown in this source by previous high angular resolution studies, which have revealed [BHB2007] 11 as a dynamic system, surrounded by a complex filamentary structure connecting to the larger circumbinary disk (2). We thus also investigate the kinematics of this source and present the first detection of a large-scale dynamic feature in this source.

Figure 1: Colour Scale: H_2CO 3(0,3)-2(0,2) centroid velocity map from pixel-by-pixel Gaussian analysis showing pixels with intensity above 5sigma in the redshifted (upper panel) and blueshifted (lower panel) regimes, overlaid with 1.3mm contours (black) and CO 2-1 outflow emission contours (red in upper panel; cyan in lower panel). The ALMA synthesised beam is in the lower left corner.

A study of the ^{13}C and ^{15}N fractionation in low-mass starless cores

Sigurd S. Jensen[1], Silvia Spezzano[1], Paola Caselli[1], Elena Redaelli[1], Olli Sipilä[1], Judit Ferrer Asensio[1] and Katharina Giers[1]

[1]*Max-Planck-Institut für extraterrestrische Physik, Giessenbachstrasse 1, D-85748 Garching, Germany*

e-mail: sigurdsj@mpe.mpg.de

Isotopic fractionation is an important diagnostic tool to study interstellar chemistry and trace the evolution of material from molecular clouds to planetary systems [1,2]. In particular, the nitrogen isotopic ratio ^{14}N/^{15}N can trace the evolution of primordial Solar System material up to the present [3]. Currently, it is unclear what physical and chemical processes determine the degree of fractionation in nitrogen-bearing species and a larger observational sample is needed. Both environmental effects, e.g., differences in irradiation and temperature, and nucleosynthetic effects are possible drivers of the fractionation [2,4]. The ^{14}N/^{15}N ratio is often determined assuming a constant ^{12}C/^{13}C ratio for simplicity (the *indirect* method). However, this assumption has been challenged by recent astrochemical models of carbon fractionation which show a significant variation in carbon fractionation in starless cores at different chemical ages and densities [5, 6]. Direct determination of both the ^{12}C/^{13}C and ^{14}N/^{15}N ratios can reveal to what extend the ^{12}C/^{13}C ratio varies in these cores and whether the indirect method remains valid while also increasing the observational sample. Deciphering the underlying processes of isotopic fractionation will provide a significant input to the study of chemical diversity during star- and planet formation as well as volatile delivery in the Solar System.

In this talk, I will present new IRAM 30m observations of HCN (1-0) and HCN (3-2) as well as H^{13}CN and HC^{15}N (1-0) toward a sample of 6 low-mass starless cores. The ^{12}C/^{13}C and ^{14}N/^{15}N ratios for HCN are directly derived through 1D line-radiative transfer modeling of the observed hyperfine emission lines. Parameter estimation is done using the Markov chain Monte Carlo method. I will present results of this analysis and compare with previous determinations of the ^{12}C/^{13}C and ^{14}N/^{15}N ratios of HCN in starless cores and discuss the implications for chemical inheritance from cores to disks and planets.

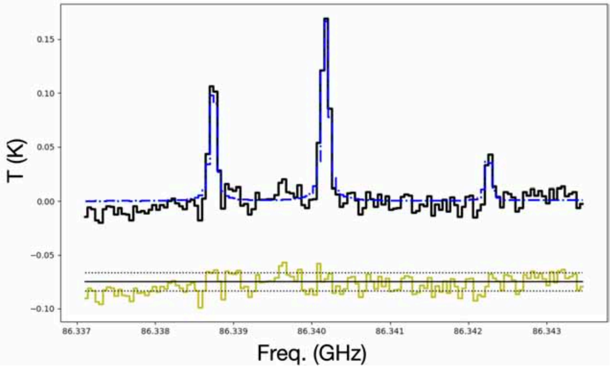


Figure 1: *Example of H^{13}CN 1-0 hyperfine emission lines fitted toward the TMC2 starless core. Yellow lines indicate the residual, offset for clarity.*

1.Caselli, P. & Ceccarelli, C. 2012, A&A Rev., 20, 56

2. Hily-Blant, P., et al. 2013a, Icarus, 223, 582

3. Wirström, E. S. & Charnley, S. B. 2018, MNRAS, 474, 3720

4. Furuya, K. & Aikawa, Y. 2018, ApJ

5. Colzi, L., et al. 2020, A&A , 640, A51 **6.** Magalhães, V. S., et al. 2018, A&A , 615, A52

Formaldehyde Deuteration In The Young Disk of IRS 63: The Astrochemical Link To The Origin Of The Solar System

Linda Podio[1] , Dominique Segura-Cox[2], and the FAUST Team

[1]*INAF - Osservatorio Astrofisico di Arcetri, Largo E. Fermi 5, 50125, Firenze, Italy*

[2] *Department of Astronomy, The University of Texas at Austin, 2515 Speedway, Austin, TX, 78712, USA*

e-mail: linda.podio@inaf.it

ALMA revolutionised our comprehension of planet formation, unveiling the presence of rings and gaps in disks, a possible signature of dust grain growth and/or young protoplanets embedded in the disk. These substructures have been detected also in the disk of the young (<500,000 years) protostar IRS 63, a Class I source located in the nearby Ophiuchus molecular cloud, suggesting that planet formation occurs early, in disks of less than 1 Myr.
In parallel, ALMA is also revolutionising our comprehension of the disk chemistry, which is crucial to understand what chemical composition planets inherit from their natal environment.

In the context of the ALMA Large Programme FAUST (Fifty AU STudy of the chemistry in the disk/envelope system of Solar-like protostars; 2018.1.01205.L, PI: S. Yamamoto), we present observations of single and doubly deuterated formaldehyde (HDCO and D_2CO) in the disk of IRS 63. Molecular deuteration is a powerful tool to trace back the history of the Solar System as the deuterium fraction in molecular species, such as formaldehyde, is enhanced in cold prestellar cores and may then be inherited by the protostellar disk and delivered to the nascent planets. We compare our estimate of the deuterium fraction in H2CO in the disk of IRS 63 with the values obtained for prestellar cores, Class 0 and I protostars, and comets, to discuss the inheritance of chemical complexity from the cold prestellar phases to young planet-forming disks.

Chemical evolution from molecular clouds to star-forming regions, and beyond

Yasuhiro Oba[1]

[1]*Institute of Low Temperature Science, Hokkaido University, N19W8, Kita-ku, Sapporo – JAPAN*

e-mail:oba@lowtem.hokudai.ac.jp

More than 200 chemical species (typically called as interstellar molecules) have been identified in the interstellar medium (ISM), and the recent great development of telescopes such as ALMA and JWST enables ones to see more real pictures of “molecular Universe”. To better understand the formation mechanisms of interstellar molecules under conditions typical in the ISM (e.g. ultrahigh vacuum at 10 K), a number of researches have been performed in laboratory. For example, most major molecules found on interstellar grains such as water and methanol can be readily synthesized by surface reactions on icy surfaces at temperatures as low as 10 K[1]. Thanks to such efforts in laboratory, our understanding on the formation of interstellar molecules is getting improved very well.

After the formation in such low-temperature environments, interstellar molecules on icy grains may have experienced further modifications by energetic particles such as cosmic rays and ultraviolet photons through the evolution of a central star, resulting in the formation of highly complex species which cannot be synthesized at low temperatures. Laboratory experiments have demonstrated that various kinds of complex organic molecules (COMs) such as amino acids, sugars, and nucleobases can be synthesized by such energetic processes from interstellar ice analogs containing water, carbon monoxide, ammonia, methanol, and/or other simple molecules, followed by warming up to room temperatures[2-4]. Although the detailed formation mechanisms of COMs still largely remain unclear, it is widely accepted that such energetic processes play a role for COMs formation in these environments[5].

So, what is the fate of these COMs formed in molecular clouds and star-forming regions? Since early 80’s, organic molecules present in carbonaceous meteorites, which are the fragments of carbonaceous asteroids in the solar system, are considered to have a contribution from chemistries in low-temperature environments such as the ISM and the outer regions of protoplanetary disks. However, there is a huge gap in terms of molecular complexity between molecules in the ISM and in meteorites; namely, the size and the variability of molecules in meteorites are far above those found in the ISM. In this talk, I would like to focus on the relationship between interstellar and meteoritic molecules based on recent studies on laboratory experiments and analyses of extraterrestrial materials including samples returned from the asteroid Ryugu.

1. T. Hama, N. Watanabe, *Chem. Rev.*, **2013**, 113, 8783-8839
2. G. M. Muñoz Caro et al., *Nature*, **2002**, 416, 403-406
3. C. Meinert et al., *Science*, **2016**, 352, 208-212
4. Y. Oba et al., *Nature Communications*, **2019**, 10, 4413
5. K. I. Öberg, *Chem. Rev.*, **2016**, 116, 9631-9663

Combined hydrodynamic and gas-grain chemical modeling of star-forming cores

M. Bonfand[1] and R. Garrod[1]

[1] *University of Virginia, Department of Astronomy, Charlottesville, VA 22904,*

e-mail: pgu4gb@virginia.edu

Astrochemical models are commonly used to predict molecular abundances to help with interpreting observational data. However, these simulations have traditionally neglected to couple the chemical evolution with a rigorous treatment of the physical evolution of the investigated source. In particular, an accurate treatment of the temperature and spatial distribution is crucial in order to run realistic simulations of star formation

I will present a new gas-grain (three-phase) chemical kinetic model[1], which reflects the most recent experimental and observational evidences for the production of complex organic molecules (COMs) both in the grain mantles at low temperature, and in the gas phase. The chemical simulations are coupled with a 2D radiation-hydrodynamic (RHD) model[2,3] that produces a set of astrochemical models that evolve according to explicitly calculated temperature, density, and spatial profiles, for a range of mass from high (final stellar mass ~23 M_{sun}) to lower mass cores (final mass < 8 M_{sun}).

With a particular focus on COMs, we aim to determine the physical and chemical origin of these species, i.e. how, where and when they form, as well as how they evolve from the protostellar envelope to the accretion disk surrounding the star (see Fig. 1).

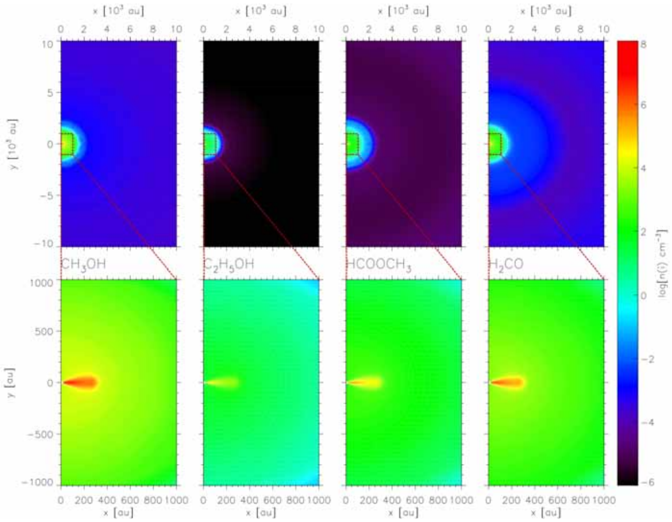


Figure 1: *Spatial distribution of the absolute abundance of four species in the envelop of a 15M_{sun} star-forming core, 12500yr after the beginning of the free-fall collapse.*

1. Garrod, R. T., Jin, M., Matis, K. A., et al. **2022,** ApJS, 259, 1
2. Barger, C. J., Lam, K. H., Garrod, R. T., et al. **2021,** A&A, 651, A43
3. Bonfand, M, Garrod, R.T, et ak. 2023 *(in prep.)*

Heterogeneous Astrocatalysis. Mechanistic Studies For The Catalytic Formation Of iCOMs Based On Fischer-Tropsch Processes.

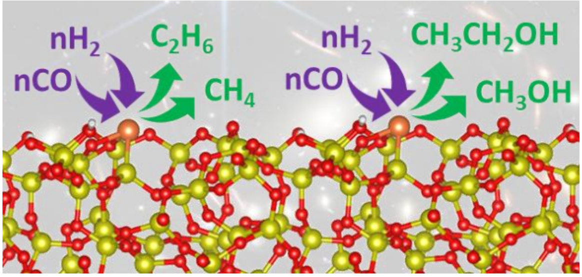
Gerard Pareras[1] & Albert Rimola[1]

[1]*Universitat Autònoma de Barcelona, Departament de Química, Barcelona, Catalunya – SPAIN*

gerard.pareras@uab.cat

Life on earth, and concretely, how the simplest organic matter not only appeared but also evolved to more complex systems is still one of the unsolved enigmas of the origin of life. The most scientifically accepted scenario assumes that the simplest organic molecules were formed over the interstellar dust during the star formation process to be later incorporated to bigger bodies. During this same process such molecules evolved to more complex ones with prebiotic relevance.[1] Nevertheless, the mechanisms from which this complexation happened are yet under debate. Recent studies shed some light to this matter as they demonstrated the presence of transition metals (TMs) incorporated within the structure of the dust.[2] Matter of fact, the discovery of the presence of TMs opens a new perspective in the branch of the Astrochemistry, the heterogeneous Astrocatalysis. Due to the relatively large abundancies of diatomic molecules such as H_2, CO and N_2, catalytical processes such as Fischer-Tropsch (FT) and Haber-Bosch (HB) are perfect candidates to convert those simple molecules to more complex ones with probiotic potential as acetaldehyde (CH_3CHO) and formamide (NH_2CHO).

In this work we provide mechanistic studies based on quantum chemistry simulations to rationalize the catalytic efficiency of the TMs, considering their different states and how they can be allocated over the dust surfaces, in this case represented as an amorphous SiO_2 model. Here, we propose the catalytic formation of different iCOMs such as, methanol, ethanol and methene from the direct coupling of carbon monoxide and molecular hydrogen. Understanding how heterogeneous catalysis can operate in the interstellar medium is a key step in providing initial data to predict catalytic processes in different stages of the planetary system formation, thus opening new and unexplored synthetic routes for the iCOMs' formation.



1. Herbst, E. Int. Rev. Phys. Chem. 2017, 36, 287–331.
2. Nuth III, J. A., Charnley, S. B. & Johnson, N. M. Meteorites Early Sol. Syst. II, 2006, 147, 147–167.

Hydrogenation Of CO, H_2CO, And CH_3CHO Alongside NO In The Interstellar Medium

J. Vitorino[1], E. Congiu[1], and F. Dulieu[1]

[1]*CY Cergy Paris Université, Observatoire de Paris, PSL University, CNRS, LERMA, 5 Mail Gay-Lussac, F-95000, Neuville-sur-Oise, FRANCE*

e-mail: julie.vitorino@cyu.fr

Nitrogen monoxide (NO) and H atoms are known to be a very reactive couple on dust grains in cold interstellar conditions[1,2,3,4]. The barrierless reaction, where the radical H_2NO plays a major role, leads in particular to ammonia (NH_3), nitrogen dioxide (NO_2), nitrous oxide (N_2O), and hydroxylamine (NH_2OH). When a third component is added to the mixture, the molecular complexity builds up, leading to some of the simplest prebiotic molecules detected.

We present a study of three different reactions involving NO and H, mixed together with either formaldehyde (H_2CO, reaction (i)), acetaldehyde (CH_3CHO, reaction (ii)), or carbon monoxide (CO, reaction (iii)), on a gold surface, with and without a water ice matrix.

Temperature programmed desorption experiments and Fourier transform infrared reflection spectroscopy were performed to analyze the reaction products and their proportions at low and high temperatures.

Three different interstellar complex organic molecules (iCOMs) were found in situ at 10K. Reaction (i) generates formamide (NH_2CHO), reaction (ii) generates acetamide (CH_3CONH_2), and reaction (iii) gives mainly isocyanic acid (HNCO). Generally, the presence of water ice favors the reactivity towards iCOMs. In reaction (ii), we demonstrated that the efficiency of the H_2NO radical is higher than that of the methyl radical (CH_3•). In reaction (iii), our findings are in accordance with several studies[2,5,6,7], regarding the propensity of formamide to return to HNCO. Lastly, our findings show that forming amide compounds seems to be easier than forming alcohol compounds.

1. E. Congiu, G. Fedoseev, S. Ioppolo, F. Dulieu, H. Chaabouni, S. Baouche, J.-L. Lemaire, C. Laffon, P. Parent, T. Lamberts, H. M. Cuppen, H. Linnartz, *The Astrophysical journal letters*. **2012**, 750(1), L12

2. F. Dulieu, T. Nguyen, E. Congiu, S. Baouche, V. Taquet, *MNRAS: Letters*. **2019**, 484(1), L119-L123

3. T. Nguyen, D. Talbi, E. Congiu, S. Baouche, A. Karton, J.-C. Loison, F. Dulieu, *ACS Earth and Space Chem.* **2019**, 3(7), 1196-1207

4. G. Fedoseev, K. J. Chuang, E. F. van Dishoeck, S. Ioppolo, H. Linnartz, *MNRAS*. **2016**, 460(4), 4297-4309

5. K. A. Haupa, G. Tarczay, Y.-P. Lee, *Journal of the Am. Chem. Society*. **2019**, 141, 11614-11620

6. J. Noble, P. Theulé, E. Congiu, F. Dulieu, M. Bonnin, A. Bassas, F. Duvernay, G. Danger, T. Chiavassa, *A&A*. **2015**, 576, A91

7. A. Lopez-Sepulcre, N. Balucani, C. Ceccarelli, C. Codella, F. Dulieu, P. Theulé, *ACS Earth and Space Chem.* **2019**, 3, 10, 2122-2137

Origin of COMs Towards Hot Cores Selected from ALMA-IMF

T. Csengeri[1] , M. Bonfand[2], L. Bouscasse[3], T. Kushwahaa and ALMA-IMF collaboration

[1] *Laboratoire d'Astrophysique de Bordeaux, Univ. Bordeaux, CNRS,*
B18N, allée Geoffroy Saint-Hilaire, 33615 Pessac - FRANCE

[2] *Department of Astronomy, University of Virginia, Charlottesville, VA 22904 – USA*

[3] *IRAM, 300 rue de la Piscine, 38400 Saint-Martin-d'Hères - FRANCE*

e-mail: timea.csengeri@u-bordeaux.fr

Complex organic molecules (COMs) are characteristic of the chemical complexification of the star forming gas, yet we still have a poor understanding about the interplay between the physical processes and the chemical evolution of the collapsing gas. In particular, the enrichment of the star forming gas in COMs is associated with deeply embedded heating sources, for precursors of high-mass stars typically referred to as hot cores. The ALMA-IMF Large program images 15 of the most prominent Galactic protoclusters over various evolutionary stages[1,2]. Beyond the rich core population uncovered by ALMA-IMF, we identified a sample of ~70 hot core candidates using CH_3OCHO lines[3]. Our main result shows that the most massive cores are all associated with CH_3OCHO emission, demonstrating that all massive cores undergo the hot core phase. Furthermore, our sample of hot core candidates exhibits emission in a variety of COMs underlying the complex chemistry associated with hot cores. Based on the non-continuous ~6.7 GHz wide frequency range of ALMA-IMF, we constrain the physical conditions, such as temperature, and the chemistry of hot cores through measures of relative molecular abundances. Using a statistical approach, we explore the diversity of COMs towards this sample of hot cores. We put in context our results with our understanding of the global molecular diversity of hot cores and hot corino like objects, and discuss the origin of COMs.

1. Motte, Bontemps, Csengeri et al., *A&A*. **2022**, 662, 8
2. Ginsburg, Csengeri, Galvan-Madrid et al., *A&A*. **2022**, 662, 9
3. Bonfand, Csengeri et al. *A&A*, **2023**, subm.

Unravelling The Path to Molecular Complexity With Quantum Chemistry

Isabelle Fourré[1,] Chloé Simha[1], Anthony Fontana[1], Riccardo Spezia[1]

[1]*Sorbonne Université, Laboratoire de Chimie Théorique, 4 place Jussieu, 75005 Paris, France* [2]

e-mail: isabelle.fourre@sorbonne-universite.fr

The subject of molecular complexification in the interstellar medium (ISM) is an active field of research, driven by the ever increasing performance of radio astronomy: indeed, of the nearly 300 molecules detected to date in the ISM, about 70 are “complex” organic molecules (COMs), i.e. with more than 5 atoms including at least one carbon atom.

However, astrochemical kinetic models sometimes struggle to reproduce the observed abundances of some COMs. This is the case for glycolonitrile ($HOCH_2CN$, discovered in 2019 toward the protostar IRAS16293-2422 B[1]), a molecule of prebiotic interest, as well as for the two most stable isomers of the H_3C_2S species, thiopropadienone H_2CCCS and thiopropynal HCSCCH (discovered with many other sulfur-bearing molecules in the cold cloud TMC-1 in 2021[2,3]). In each case the lack of gas-phase reactions in the chemical reaction network was pointed out by the authors of the detections.

Quantum chemistry is one of the pillars of “laboratory astrophysics”, together with spectroscopy and study of chemical reactions under extreme conditions of pression and temperature: as such, it is a valuable tool for unravelling the reaction formation and destruction processes of COMs. The harsh conditions in the molecular clouds, with number densities ranging between 10^2 and 10^7 cm^{-3} and temperatures varying from 10 K to 150 K, severely constrain the chemical reactivity. Indeed, due to low temperatures, reactions should start with a barrierless attack, and proceed with only submerged barriers (unless a tunnelling is possible). Moreover, in the gas phase, due to the extremely low densities, only bimolecular reactions occur and two species should be produced, one of which taking away the excess energy (radiative stabilization being an exception)[4].

In spite of these constraints, viable reactions mechanisms in the gas phase of the ISM can be established with state-of the-art quantum chemistry calculations. I will show some results for radical + neutral and ion + neutral reactions leading to the formation of the previously mentioned molecules (Figure 1).

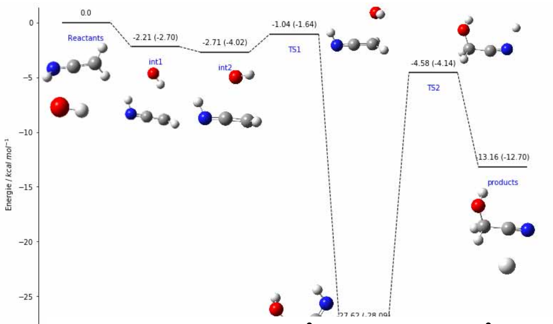


Figure 1 : $CH_2CNH + OH^{\bullet} = HOCH_2CN + H^{\bullet}$

(1) Zeng, S. et al. R. *Mon. Not. R. Astron. Soc. Lett.* **2019**, *484* (1), L43–L48.
(2) Cernicharo, J. et al. *Astron. Astrophys.* **2021**, *648*, L3.
(3) Cernicharo, J. et al. *Astron. Astrophys.* **2021**, *650*, L14.
(4) Puzzarini, C. *Front. Astron. Space Sci.* **2022**, *8*, article 811342.

Unveiling chemical structures of star-forming regions with machine learning techniques

Katharina Giers[1] , Silvia Spezzano[1], Yuxin Lin[1], and Paola Caselli[1]

[1]*Max-Planck Institute for Extraterrestrial Physics, Centre for Astrochemical Studies, Giessenbachstrasse 1, Garching – GERMANY*

e-mail: kgiers@mpe.mpg.de

The distribution and abundance of molecules provide information on the chemical and physical structures in cold and dense cores[1,2], where star formation takes place. This helps to gain understanding on the star formation process itself[3], and subsequently on the planet and planetary system formation[4]. In particular the earliest stages of star formation, where the protostar has not yet been formed, play an important role. There, the chemistry and physics can be studied without complications caused by the protostellar feedback. Molecular line emission maps are a powerful tool to study the molecular cloud structure, e.g. giving information on volume density or gas temperature[1,5]. Starless cores provide the initial budget that will eventually form planets. Therefore, understanding their chemistry is crucial to understand what happens next.

We have undertaken a survey of molecular line emission maps in starless and pre-stellar cores. We cover 34 molecular lines towards seven sources, observed with the IRAM 30m single-dish radio telescope. To analyse the large dataset, we use different statistical methods and unsupervised clustering algorithms. With this, we are able to study the chemical differentiation and complexity in the observed cores, revealing the different physical and chemical phases present.

In my talk, I will discuss the behaviour of the observed molecules in the cores in our sample and the influence of the environment, including different illuminations, on their emission morphology. In addition, we investigate the segregation between the molecules in each of the cores separately. I will discuss the correlations among different molecules and their dependence on physical parameters of the core, linking chemical and physical structures by building detailed physical models of the cores.

1. A. Crapsi, P. Caselli, M. C. Walmsley, M. Tafalla, *A&A*, **2007**, 470, 221-230
2. Y. Lin, S. Spezzano, O. Sipilä, A. Vasyunin, P. Caselli, *A&A*, **2022**, 665, 22
3. E. Keto, P. Caselli, J. Rawlings, *MNRAS*, **2015**, 446, 3731-3740
4. M. N. Drozdovskaya, I. R. H. G. Schroeder, M. Rubin, K. Altwegg, E. F. van Dishoeck, B. M. Kulterer, J. De Keyser, S. A. Fuselier, M. Combi, *MNRAS*, **2021**, 500, 4901-4920
5. E. Redaelli, O. Sipilä, M. Padovani, P. Caselli, D. Galli, A. V. Ivlev, *A&A*, **2021**, 656, 16

A Spatially Resolved Map of Cosmic Ray Ionization Rate and Electron Fraction

Jaime E Pineda[1] , O. Sipilä[1], D. M. Segura-Cox[2], R. Neri[3], M. Kuffmeier[4,1], M. T. Valdivia-Mena[1], M. J. Maureira[1], P. Caselli[1], S. Spezzano[1], S. S. R. Offner[2], N. Cunningham[5], A. Schmiedeke[6], and M. Chen[7]

[1] *Max-Planck-Institut für extraterrestrische Physik, Giessenbachstrasse 1, 85748 Garching, Germany*

[2] *Astronomy Department, The University of Texas at Austin, 2500 Speedway, Austin, TX 78712, USA*

[3] *IRAM, 300 rue de la Piscine, F-38406, Saint- Martin d'Hères – France*

[4] *Department of Astronomy, University of Virginia, Charlottesville, VA, 22904 – USA*

[5] *IPAG, Université Grenoble Alpes, CNRS, F-38000 Grenoble – France*

[6] *Green Bank Observatory, PO Box 2, Green Bank, WV 24944 – USA*

[7] *Department for Physics, Engineering Physics and Astrophysics, Queen's University, Kingston, ON, K7L 3N6, Canada*

e-mail: jpineda@mpe.mpg.de

Electron fraction and cosmic ray ionization rates in star-forming regions are important quantities controlling the chemical complexity in dense cores and to properly quantify non- ideal MHD terms. However, these are difficult quantities to estimate. We combined observations of the nearby NGC 1333 star-forming region carried out with NOEMA interferometer and 30m single dish to generate high spatial dynamic range maps of different molecular transitions. We use the ratio of DCO^+ and $H^{13}CO^+$ (in addition to complementary data) to estimate the electron fraction and cosmic ray ionization rate maps.

We derive the first electron fraction and cosmic rate ionization rate maps in a star- forming region. The maps present clear evidence for interaction with a single nearby bubble, as previously suggested. We find high values of the electron fraction, as well as strong evidence for locally generated cosmic rays. We show how a higher cosmic ray ionization rate (compared to the canonical value of 10^{-17} s^{-1}) is found in the region, and it is generated by the accreting young stellar objects. Moreover, the electron fraction is affected by the depletion of metals and the higher cosmic rate in these regions.

I will discuss further implications and opportunities to expand these studies.

The chemical composition of solar-type protostars with the ALMA large spectral surveys PILS and COMPASS

Audrey Coutens[1], the PILS team and the COMPASS team

[1]*Institut de Recherche en Astrophysique et Planétologie (IRAP), Université de Toulouse, UPS-OMP, CNRS, CNES, 9 av. du Colonel Roche, F-31028 Toulouse Cedex 4, France*

e-mail: audrey.coutens@irap.omp.eu

Complex organic molecules easily form in star-forming regions. Those present in the inner regions of solar-type protostars could be incorporated into comets and asteroids before being delivered into planets through impacts. They could then potentially play a role in the emergence of life if the conditions on the planets are suitable. Large unbiased spectral surveys are ideal to characterize the molecular content of star-forming regions. An ALMA large spectral survey (PILS[1]) was carried out a few years ago towards the solar-type protostar IRAS 16293-2422, which allowed us to determine the chemical composition of this source. To determine if IRAS 16293-2422 is representative of all solar-type protostars, the chemistry of more sources needs to be investigated. The ALMA large program COMPASS has for aim to answer this question. In this talk, I will present some of the main results of the PILS program as well as the objectives of the COMPASS large program.

1. J. K. Jørgensen, M.H. D. van der Wiel, A. Coutens et al. 2016 A&A 595, A117

Dimerization of HCN on Interstellar Silicates Grain Cores: A Quantum Mechanical Study

Niccolò Bancone[1,2], Stefano Pantaleone[2], Piero Ugliengo[2], Marta Corno[2], Albert Rimola[1]

[1]*Universitat Autònoma de Barcelona, Departament de Química, E-08193, Bellaterra – SPAIN*

[2] *Università degli Studi di Torino, Dipartimento di Chimica, I-10125, Torino – ITALY*
e-mail: niccolo.bancone@uab.cat

Hydrogen cyanide (HCN) has been receiving an increasing attention as a possible precursor of life since when J. Orò synthesized adenine from a solution of HCN and ammonia.[1] Since HCN molecules are widespread in the interstellar medium and the products of its polymerization (including purines) have been detected on meteoritic fragments,[2] the scientific community is now investigating the possible pathways for the oligomerization of HCN in cosmic environments to form molecules of prebiotic interest. In this sense, the gas phase oligomerization of HCN is hindered by high energetic barriers which cannot be overcome at the conditions of a molecular cloud.[3] In the condensed phase, instead, more promising results were obtained, thanks to a more feasible acid-base chemistry.[4]

For these reasons, the surfaces of interstellar dust grains, as well as other materials such as carbonaceous chondrites and cometary nuclei, may play a fundamental role in this type of chemistry. Moreover, it has been recently demonstrated that the surfaces of silicates, among the primary components of dust grains cores, are able to catalyze the oligomerization of HCN to adenine.[5]

In this work we investigated the dimerization of two HCN molecules adsorbed on crystalline Mg_2SiO_4 (forsterite) surfaces with the formation of iminoacetonitrile ($H_2C_2N_2$). By modelling five dimerization cases on three different surfaces, we observed that, thanks to their acid-base properties,[6] forsterite surfaces are able to deprotonate one adsorbed HCN molecule, triggering the reaction, and to stabilize the transition states of iminoacetonitrile formation. Most cases show favorable energetic barriers and, according to a kinetic analysis, the reaction is likely to take place at the conditions proper of proto-planetary disks and planetesimals formation, while it results to be hindered in molecular clouds.

1. J. Orò, *Nature*, **1961**, 191, 1193-1194
2. Z. Martins, *et al.*, *Orig. Life Evol. Biosph.*, **2009**, 39, 214
3. I. W. M. Smith, D. Talbi, E. Herbst, *Astron. Astrophys.*, **2001**, 369, 611-615
4. O. Kikuchi, T. Watanabe, Y. Satoh, Y. Inadomi, *J. Mol. Struct. THEOCHEM,* **2000**, 507, 53-62
5. R. Santalucia *et al.*, *Phys. Chem. Chem. Phys.*, **2022**, 24, 7224-7230
6. M. Signorile, *et al., ACS Earth Space Chem.*, **2020**, 4, 3, 345-354

Astrochemically Relevant H-Atom-Abstraction and H-Atom-Addition Reactions Connecting Fulminic Acid (HCNO) and Formaldoxime (H_2CNOH)

Barbara Keresztes[1,2], Sándor Góbi[3], István Pál Csonka[3], Gopi Ragupathy[3],
Gábor Bazsó[4], and György Tarczay[1,3,5]

[1]*Laboratory of Molecular Spectroscopy, Institute of Chemistry, ELTE Eötvös Loránd University, P.O. BOX 32, H-1518 Budapest – HUNGARY*
[2]*Hevesy György PhD School of Chemistry, Institute of Chemistry, ELTE Eötvös Loránd University, P.O. BOX 32, H-1518 Budapest – HUNGARY*
[3]*MTA–ELTE Lendület Laboratory Astrochemistry Research Group, Institute of Chemistry, ELTE Eötvös Loránd University, P.O. BOX 32, H-1518 Budapest – HUNGARY*
[4]*Wigner Research Centre for Physics, P.O. BOX 49, H-1525 Budapest – HUNGARY*
[5]*Centre for Astrophysics and Space Science, ELTE Eötvös Loránd University, P.O. BOX 32, H-1518 Budapest – HUNGARY*
e-mail: barbi1226@gmail.com

Today one of the central questions of astrochemistry is how H_2 is formed in dense molecular clouds. Because of the low pressure in the interstellar medium the possibility of the 3-body-collisions is low, which means that the H_2 cannot be formed from 2 H-atoms in gas phase. According to recent theoretical studies it is possible that H_2 is generated in catalytic cycles[1]. In the catalytic cycles two H atoms forms an H_2 molecule not directly but with the help of a catalyst.

The aim of our research work was to investigate the catalytic cycle of fulminic acid (HCNO) and formaldoxime (H_2CNOH). The molecules were trapped in *para*-H_2 matrix at 3.1 K. Then, H atoms were generated in the matrix. In *para*-H_2, the H atoms can diffuse efficiently by tunnel effect, which enabled the examination of its reactions (H-atom-addition and H-atom-abstraction reactions) with the trapped molecules. The chemical changes were followed by IR spectroscopy.

According to our experimental results, HCNO and H_2CNOH can react with H atoms at 3.1 K. This observation indicates that the same reactions might also occur at 10−20 K in the dense molecular clouds which means that these reactions can catalyze the H_2 formation in the ISM. The experimental results have shown that the quantity of HCNO and H_2CNOH is connected to each other through a quasi-equilibrium reaction. This quasi-equilibrium is shifted towards the HCNO, which may explain why H_2CNOH has not been detected yet in the ISM.

1. Vidali, G., *Chemical Reviews* **2013**, 12, 8762-8782

Protostellar shocked regions as factories of organic molecules: the case of L1157

Ana López-Sepulcre[1,2], Claudio Codella[3,1], Linda Podio[3], Cecilia Ceccarelli[1], Nadia Balucani[4]

[1]*Univ. Grenoble Alpes, CNRS, IPAG, 38000 Grenoble – FRANCE*

[2] *Institut de Radioastronomie Millimétrique, 38406 Saint-Martin d'Hères – FRANCE*

[3]*INAF, Osservatorio Astrofisico di Arcetri, Largo E. Fermi 5, I-50125, Firenze - ITALY*

[4]*Dipartimento di Chimica, Biologia e Biotecnologie, Universit`a degli Studi di Perugia, 06123 Perugia - ITALY*

e-mail: ana.lopez-sepulcre@univ-grenoble-alpes.fr, lopez@iram.fr

Life on Earth is known to be very diverse. And yet, its basic ingredients are always the same: organic molecules with varying degrees of complexity. Interestingly, simplified versions believed to be building blocks of such organic molecules can be observed in regions where stars and planets are forming today in our Galaxy. This can help us understand their chemistry along the different evolutionary phases leading to a star and planetary system like our own. Still, we are far from achieving a full comprehension of how organic chemistry works in space.

In this context, protostellar shocks are particularly well-suited to study the formation and destruction pathways of organic molecules, since the sputtering and shattering of dust grains release atoms and molecules previously settled in the dust grain cores and mantles into the gas phase. This triggers a rich and relatively warm chemistry that evolves over time. An illustrative example is the molecular outflow driven by the protostar L1157, which creates several chemically-enriched shocked regions along its path. I will present the results from interferometric observations of various organic molecules such as formamide (NH_2CHO), acetaldehyde (CH_3CHO), methanol (CH_3OH), and ethanol (C_2H_5OH), along the entire southern outflow lobe driven by the L1157 protostar, which we carried out with the NOEMA (Northern Extended Millimetre Array). The molecular maps cover three main shocked regions with different ages, which, combined with astrochemical modelling, allows us to assess the time evolution of the targeted organic molecules' chemistry. Based on our results, I will show the importance of gas-phase chemistry in the production of formamide and other organic molecules in protostellar shocks.

Super-Oxygenation of Naphthalene: The break-Down Reaction

Dario Campisi[1]

[1]*University of Stuttgart, Institute for Theoretical Chemistry, Pfaffenwaldring 55, Stuttgart – GERMANY*

e-mail: campisi@theochem.uni-stuttgart.de

Polycyclic aromatic hydrocarbons (PAHs) are interstellar molecules ubiquitous in the Universe that lock up ~15% of the C in space. If this C can be made available, it may play a role in the formation of complex organic molecules (COMs)[1]. While COM formations start with the activation of CO through hydrogenation reactions, the break-down reaction of PAHs may provide an alternative route for COM formations in space[1]. Atomic O has an abundance of ~10^{-4} with respect to atomic H and 35% of O abundance is missing in cold regions of interstellar medium (ISM) with respect to the total O abundance in the ISM[2]. If atomic O binds with PAHs, it might contribute to form COMs and, thus, this might explain the lack of O abundance. PAHs are known to react with atomic H becoming super-hydrogenated[3]. However, studies on the reaction of PAHs with atomic O are currently missing.

Here, using density functional theory (DFT), I predicted the formation of possible intermediates of the reaction of atomic O with naphthalene (Fig. 1). DFT calculations predict O attachment sequence equal to the first hydrogenation of naphthalene[4]. The energy barrier for the first O attachment is 0.13 eV, which is lower than the first H attachment in PAHs such as coronene[5] (0.19 eV) and pyrene[6] (0.22 eV). Once atomic O reacts with the first C atom of naphthalene, intersystem crossing (ISC) occurs from the triplet to the singlet spin state. In the singlet state, the O will bridge two adjacent carbon atoms of the naphthalene. The resulting O bridge catalyzes the barrier-less break-down reaction of the C-C bond that the O is bridging, forming a seven-membered heterocyclic ring. A second O radical will bind onto the adjacent carbon atom bound with the first O atom, which barrier-less breaks the C-O bond catalyzing the opening of the aromatic ring. The second oxygenation causes the loss of the PAH structure, which is the first step to understand the formation of PAH's daughters that contribute to form COMs in star-forming regions. COMs are important reagents for the formation of building blocks of life[1]. The results of this work might also explain the lack of 35% of O observed in the ISM[2].

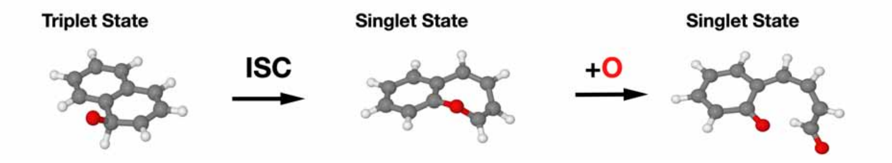


Figure 1: *Super-Oxygenation (in red) of naphthalene leading to opening the aromatic ring.*

1. A. G. G. M. Tielens, *Rev. Mod. Phys.* **2013**, 85, 1021
2. D. C. Lis *et al.*, *A&A* **2023**, 669, L15
3. D. Campisi *et al.*, *Phys. Chem. Chem. Phys.* **2020**, 22, 1557-1565
4. B. Klærke *et al.*, *A&A* **2013**, 549, A84
5. P. A. Jensen *et al.*, *MNRAS* **2019**, 486, 5492-5498
6. D. Campisi *et al.*, Phys. Chem. Chem. Phys. **2020**, 22, 6738-6748

The Effect Of Metallicity On The Abundances Of Molecules In Protoplanetary Disks

Presenting author* , Rodrigo Guadarrama*,[1], Eduard I. Vorobyov[1,2]
, Christian Rab[3] , Manuel Güdel[1]

[1]*University of Vienna , Department of Astrophysics, Türckenschanzstrasse 17, Vienna – Austria*

[2] *Research Institute of Physics, Southern Federal University, Rostov-on-Don, 344090 – Russia*

[3]*Max-Planck-Institut für extraterrestrische Physik , Giessenbachstrasse 1, 85748 Garching – Germany*

e-mail: presenting rodrigo.guadarrama@univie.ac.at

Diverse studies have shown that it is important to consider the impact of metallicity on the chemodynamical evolution of protoplanetary disks. It has been suggested that there may be different chemistry cycles in non-solar metallicity environments at work or that the efficiency of mass transport in protostars and pre-main-sequence stars is dependent on metallicity to a certain extent.

We study the influence of different metallicities on the physical, thermal, and chemical properties of protoplanetary disks, particularly with regard to the formation and destruction of carbon-based molecules. With the thermo-chemical code PRODIMO[1] (PRotoplanetary DIsk MOdel), we investigated the impact of lower metallicities on the radiation field, disk temperature, and the abundance of different molecules (H2O, CH4, CO, CO2, HCN, CN, HCO+, and N2H+).

Our results demonstrate a relation between the metallicity of the disk and the strength of the stellar radiation field inside the disk (see Figure 1.). As the metallicity decreases, the radiation field is capable of penetrating deeper regions of the disk. This triggers among other things, a series of changes in the chemical formation and destruction efficiencies for different chemical species. Metallicity has a clear impact on the snowline of the molecules studied here as well.

We find that chemical reactions responsible for the destruction and formation of the studied molecules change as the metallicity of the disk is reduced. We found a strong overabundance (relative to scaled-down values) in the models with lower metallicity for gaseous species (CN, CO, HCO+, N2H+), which are particularly useful in observations. This could be advantageous for future observations in low-metallicity environments. Future studies ought to consider other processes, such as different dust grain size distribution, different stellar radiation fields, and stellar burst scenarios.

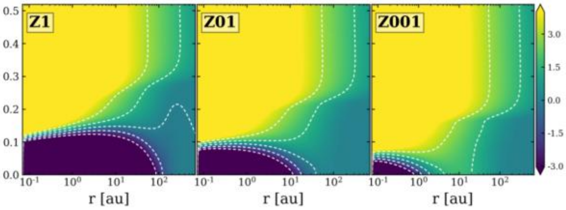


Figure 1: *UV radiation field for the fiducial model (left panel), reduced metallicity by a factor of 10 (middle panel),and by a factor of 100 (right panel), in units . The decreasing metallicity enables the UV radiation to get to the midplane at a smaller radius.*

Where Planetary Systems Are Born Matters: The Chemistry Of Clustered Versus Isolated Environments And Cradle Of The Sun

M. Bouvier[1,2], C. Ceccarelli[2], A. López-Sepulcre[2,3], N. Sakai[4], S. Yamamoto[5], Y.-L. Yang[6,4]

[1]*Leiden Observatory, Leiden University, P.O. Box 9513, 2300 RA, Leiden, The Netherlands*

[2]*Univ. Grenoble Alpes, CNRS, IPAG, 38000 Grenoble, France*

[3]*Institut de Radioastronomie Millimétrique (IRAM), 300 rue de la Piscine, F-38406 Saint-Martin d’Hères, France*

[4]*RIKEN Cluster for Pioneering Research, Wako-shi, Saitama, 351-0198, Japan*

[5]*Department of Physics, The University of Tokyo,7-3-1, Hongo, Bunkyo-ku, Tokyo 113-0033, Japan*

[6] *Department of Astronomy, University of Virginia, Charlottesville, VA 22904, USA*

e-mail: bouvier@strw.leidenuniv.nl

Stars form commonly in clusters[1]. Our Sun was likely born in a relatively large and dense one, near massive stars ($M>8M_{\odot}$)[2,3]. It is then highly probable that this clustered environment influenced several properties of the Solar System, including its early age chemical nature. To date, studies of solar-like protostars in high-mass star-forming regions (SFRs) are still too scarce compared to low-mass SFRs. It is thus crucial to increase the number of studies on Sun-like birth regions to shed light on our Sun’s past.

In this context, the ORion ALMA New GEneration Survey (ORANGES)[4] aimed to study a sample of protostars located in the Orion Molecular Clouds 2/3 (OMC-2/3) filament, the nearest high-mass SFR, to (1) have a first census of the chemical content of protostars born in a solar-like birth environment, and (2) investigate whether the highly UV-illuminated region affects the source’s chemical properties. The comparison with the analogous survey in the Perseus low-mass SFR (PEACHES: PErseus ALMA CHEmistry Survey[5]) showed that hot corinos are less abundant in Orion than in Perseus (30% against 60%), suggesting an influence of the environment on the source’s chemical structure.

In the same vein, outflows are powerful feedback processes linking the sources to their environment. Their study provides a direct measure of how the environment influences the star formation process and, specifically, its chemistry. Using ALMA and NOEMA high angular resolution observations, we could study and characterise the particularly outstanding outflow from an ORANGES source, OMC-2 FIR6c-a. Indeed, not only Methanol is observed extending over a large area but Formamide and Acetaldehyde, much rarely detected iCOMs in outflows, are also present. The analysis of each iCOM emission distribution is a powerful and almost unique tool to understand the chemical processes taking place in crowed Solar-type SFRs.

1. C. J. Lada & E. A. Lada, *ARA&A*. **2003**, 41, 57
2. 2. F. C. Adams, *ARA&A*. **2010**, 48, 47
3. S. Pfalzner & K. Vincke, *ApJ*. **2020**, 897, 60
4. M. Bouvier, C. Ceccarelli, A. López-Sepulcre, et al., *ApJ*. **2022**, 929, 1
5. Y.-L. Yang, N. Sakai, Y. Zhang, et al., *ApJ*. **2021**, 910, 20

Collision Induced Dissociation of Water Pyrene Molecular Clusters

A. Nair[1,2], S. Zamith[1], L. Toucouere[3], H. Leboucher[3], A. Simon[3], A. Marciniak[1], J.M. L'Hermite[1], C. Joblin[2]

[1] *LCAR, FERMI; Université de Toulouse (UT3); CNRS; F-31062 Toulouse, France*
[2] *IRAP, Université de Toulouse (UT3); CNRS; CNES; F-31028 Toulouse, France*
[3] *LCPQ, FERMI; Université de Toulouse (UT3); CNRS; F-31062 Toulouse, France*

Email : arya.nair@irsamc.ups-tlse.fr

In photodissociation regions (PDRs) associated with star formation, the matter composed of gas and tiny dust particles is in strong interaction with the ultraviolet (UV) radiation from young stars. From previous infrared space missions such as the Spitzer telescope, we have observed the destruction of very small carbonaceous grains and the production of isolated polycyclic aromatic hydrocarbons (PAHs) at the edge of these PDRs [1]. Clusters of PAHs have been proposed as models for these carbonaceous nanograins [2]. Furthermore, these nanograins come from the inner part of interstellar clouds where models predict a transition from gaseous to icy water [3]. Therefore, in order to get insight into the interaction of water with the carbonaceous nanograins we are performing experiments on water-PAH molecular clusters.

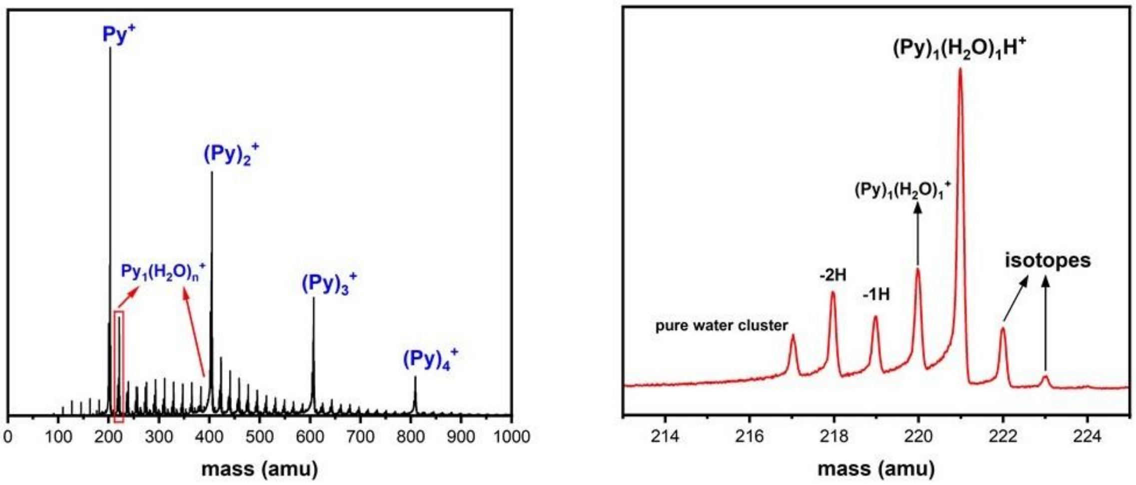


Figure 1: *Mass spectrum of cationic water pyrene clusters*

Cations of mixed water pyrene ($C_{16}H_{10}$, Py) clusters are produced in a gas aggregation source cooled at liquid nitrogen temperature [4] prior to thermalization at 25K (see example in Figure 1). Mixed clusters with up to 4 pyrene molecules and several water molecules attached can be produced with dominance of protonated species. In order to study the energetics of specific species and get insights into their structure, we record absolute fragmentation cross sections using collision induced dissociation (CID). The species of interest are mass selected and undergo collisions with inert gases at varying kinetic energy of the ions. The products are analysed by time-of-fight mass spectrometry.

CID experiments were performed on $(Py)_m(H_2O)_nH^+$ (m= 1 to 3, n= 1 to 10) and $(Py)_1(D_2O)_nD^+$ (n= 1 to 9) at 7.5 eV centre-of-mass collision energy. Both water loss and pyrene loss channels are observed. For $(Py)_1(D_2O)_nD^+$, we could also observe contribution from H-D exchange. Calculations were performed to obtain structural and energetic data and support the analysis of the experimental results in terms of proton localization and dissociation energies. Ultimately our aim is to understand how the proton localization affects the fragmentation. The results obtained so far will be presented.

[1] P. Pilleri, J. Montillaud, O. Berné, and C. Joblin, Astron. & Astrophys. 542, A69 (2012).
[2] M. Rapacioli, C. Joblin, and P. Boissel, Astron. Astrophys. 429, 193–204 (2005).
[3] D. Hollenbach, M. J. Kaufman, E. A. Bergin, G. J. Melnick, Astrophys. J. 690, 1497 (2009).
[4] I. Braud, S. Zamith, and J.-M. L'Hermite, Rev. Sci. Instrum. 88, 043102 (2017).

POSTERS

A Computational Study of the Reaction between N(^{2}D) and Simple Aromatic Hydrocarbons

Marzio Rosi,[1] Nadia Balucani,[2] Adriana Caracciolo,[2] Piergiorgio Casavecchia,[2]
Dimitrios Skouteris,[3] Gianmarco Vanuzzo[2]

[1] *University of Perugia, Department of Civil and Environmental Engineering, Via G. Duranti, 93, 06125 Perugia, ITALY*

[2] *University of Perugia, Department of Chemistry, Biology and Biotechnologies, Via Elce di Sotto, 8, 06123 Perugia, ITALY*

[2] *Master-Tec s.r.l., Via Sicilia, 41, 06128, Perugia, ITALY*

e-mail: marzio.rosi@unipg.it

Atomic nitrogen in its ^{4}S ground state exhibits very low reactivity with closed shell molecules, while in its first electronically excited ^{2}D state shows a significant reactivity with hydrocarbons. N(^{2}D) was detected in the water-poor comet C/2016 R2 (Pan-STARRS)[1] and in a plethora of strongly photon-irradiated environments including the Orion Nebula (M42), low-ionization H II regions (M43), planetary nebulae (*i.e.* the Ring Nebula), supernova remnants (*i.e.* the Crab Nebula), and Herbig-Haro objects.[2] Polycyclic aromatic hydrocarbons (PAHs) and related species are presumed to be omnipresent in the interstellar medium (ISM) and aromatic chemistry is widespread in the earliest stages of star formation.

In this contribution, we report on a theoretical characterization of the reaction involving N(^{2}D) and simple aromatic hydrocarbons, like benzene or toluene. We have already investigated the reactions of atomic nitrogen in its excited ^{2}D state with various aliphatic hydrocarbons, like CH_4, C_2H_2, C_2H_4, C_2H_6, in laboratory experiments by the crossed molecular beam technique with mass spectrometric detection and time-of-flight analysis at different collision energies complemented by electronic structure calculations of the stationary points along the minimum energy path and kinetics calculations. The aim is to determine the chemical behavior of N(^{2}D) with aromatic species after the previous investigation with aliphatic molecules. In particular, we wish to establish whether the aromatic ring is preserved in this reaction and whether the N atom is incorporated in the ring of carbon atoms.

1. S. Raghuram, D. Hutsemékers, C. Opitom, E. Jehin, A. Bhardwaj, J. Manfroid, *Astron. Astrophys.* **2020**, 635, A108

2. G. J. Ferland, W. J. Henney, C. R. O'Dell, R. L. Porter, P. A. M. van Hoof, R. J. R. Williams, *Astrophys. J.* **2012**, 757, 79. M. A. Dopita, D. J. Mason, W. D. Robb, *Astrophys. J.* **1976**, 207, 102. G. J. Ferland, M. J. Rees, *Astrophys. J.* **1988**, 332, 141. M. A. Bautista, *Astrophys. J.* **1999,** 527, 474.

An ALMA Study Of The Complex Organic Molecules Towards The Warm Planet-Hosting Disk HD 100546

Lucy Evans[1] , Catherine Walsh[1], and Alice Booth[2]
(on behalf of the proposal team)

[1]*School of Physics and Astronomy, University of Leeds, Leeds LS2 9JT - UK*

[2] *Leiden Observatory, Leiden University, PO Box 9513, 2300 RA Leiden - THE NETHERLANDS*

e-mail: l.e.evans@leeds.ac.uk

It is well established that the building blocks of prebiotic molecules present in the Solar System are already present at the earlier stages of stellar evolution (1). The protoplanetary disk HD 100546 shows strong evidence of this chemical inheritance at play; as a warm Herbig Ae/Be disk, the gas-phase methanol detected was likely not formed in situ and was therefore inherited from ices formed in the original molecular cloud (2). This is because the disk is too warm (> 20 K) to host a substantial CO ice reservoir and methanol forms efficiently only via hydrogenation of CO ice (3). As the simplest example of a complex organic molecule (COM), methanol acts as a gateway to the more complex chemistry required for the formation of pre-biotic molecules.

We present preliminary images and analysis from ALMA Cycles 7 and 8 (PI: A Booth) of the organic molecules, formaldehyde and methanol, observed towards HD 100546 at high spatial resolution (~ 0.2 arcseconds or ~ 20 au). The images show two components: one more centrally compact and coincident with the bright inner dust ring and a second, more diffuse ring, aligned with an outer dust ring. These images suggest alignment of the ice reservoir with the dust, and point to two distinct desorption mechanisms in the inner versus outer disk. With this data, we aim to constrain the distribution of these molecules in the disk as well as the desorption processes at play. Our results will provide a clearer picture of the chemical processing of these precursor molecules at planet-forming scales and will therefore lead to conclusions surrounding the development of habitable environments both in our native Solar System and also in the exoplanetary systems beyond.

1. P. Caselli & C. Ceccarelli. *A&A Rev.* **2012**, 20, 56
2. A. S. Booth, C. Walsh, J. T. van Scheltinga, E. F. van Dishoeck, J. D. Ilee, et al. *Nature Ast.* **2021**, 5, 684-690
3. S. D. Rodgers & S. B. Charnley. *Planet. Space Sci.* **2002**, 50, 1125

ATOMIS, an ALMA Archive Tool for Molecular Investigations in Space

Sahar Ben-Hmida[1], Audrey Coutens[1], and Jean-Michel Glorian[1]

[1]*Institut de Recherche en Astrophysique et Planétologie (IRAP), Université de Toulouse, UPS-OMP, CNRS, CNES, 9 av. du Colonel Roche, F-31028 Toulouse Cedex 4, France*

e-mail: audrey.coutens@irap.omp.eu

ATOMIS (ALMA archive TOol for Molecular Investigations in Space) is a web application that aims to search for specific molecular species in the observations of the ALMA archive. With ATOMIS, the user can select the sources and species of interest while specifying filters on the minimum and maximum E_{up}, A_{ij}, the uncertainty on the frequencies of the transitions. Classic filters on observations (angular resolution, spectral resolution, sensitivity, ...) are available. From ATOMIS, it is also possible to download ALMA data products such as fits cubes and visualize them using the ALADIN (http://aladin.u-strasbg.fr/) and CASSIS (http://cassis.irap.omp.eu) softwares.

Chemical Evolution by UV and Thermal Processing of COMs-Based Ices

C. del Burgo-Olivares[1] , H. Carrascosa[1], and G. M. Muñoz Caro[1]

[1]*Centro de Astrobiología, (CSIC-INTA), Ctra. De Ajalvir, km 4,Torrejón de Ardoz – SPAIN*

e-mail: cdelburgo@cab.inta-csic.es

In the colder regions of molecular clouds ice mantles are formed on dust grains. These ice mantles are mainly composed of simple volatile molecules. The ultraviolet processing undergone by these ices produces photochemical reactions that can lead to the formation of increasingly more complex molecules[1]. The increase in temperature of the ice, e.g. in hot cores, causes the desorption of these molecules to the gas phase, which can then be detected by astronomical observations. Understanding the photochemistry and desorption that take place in ices is essential for interpreting the abundances obtained from astronomical observations[2].

In our experiments we have studied the behavior of complex organic molecules (COMs) in the ice submitted to UV radiation and thermal processing. Exposure of these species (acetic acid CH_3COOH, methanol CH_3OH, and methylamine CH_3NH_2) to UV radiation leads to the formation of photoproducts. Molecules such as CO, CO_2, CH_4, H_2CO, $HCONH_2$, $CH_3CH_2NH_2$, and the N-heterocycle hexamethylenetramine ($(CH_2)_6N_4$), referred to as HMT, are obtained in our experiments. A residue remains at room temperature that is now under study.

The experiments have been performed in ISAC, an ultra-high vacuum chamber with a base pressure of 4×10^{-11} mbar and temperature down to 8 K where MgF_2/KBr substrates were used for ice deposition, reproducing the conditions of dense interstellar clouds. The ices are irradiated with a microwave discharged hydrogen lamp[3]. Reaction products in the ice were identified by infrared spectroscopy in transmittance, and gas phase molecules were detected during temperature programmed desorption monitored using a quadrupole mass spectrometer.

.

1. H. Carrascosa, C. González Díaz, G. M. Muñoz Caro, P. C. Gómez, M. L. Sanz, *MNRAS.* **2021**, 506, 791-805.
2. G. M. Muñoz Caro, A. Ciaravella, A. Jiménez-Escobar, C. Cecchi-Pestellini, C. González-Días, Yu-Jung C. *ACS Earth and Space Chemistry.* **2019**, 3 (10), 2138-2157.
3. G. M. Muñoz Caro, A. Jiménez-Escobar, J. Á. Martín-Gago, C. Rogero, C. Atienza, S. Puertas, J. M. Sobrado, J. Torres-Redondo. *A&A.* **2010**, 522, A108.

Chemical Pathways of Sulfur Bearing Species with Hydrogen Atoms without External Energies on Interstellar Ice

Thanh Nguyen[1], Yasuhiro Oba[1], W. M. C. Sameera[1,2], Akira Kouchi, and Naoki Watanabe[1]

[1]*Hokkaido University, Institute of Low Temperature Science, N19W8, Kita-ku, Sapporo – JAPAN*

[2] *University of Colombo, Colombo – SRI LANKA*

e-mail: presenting nguyenthanh@lowtem.hokudai.ac.jp

There have been about 30 sulfur (S)-bearing species identified in the interstellar medium (ISM). Since the observed abundance of S-bearing species in the gas phase is lower than the cosmic abundance of S[1], it is often considered that there might be a source of “missing S" on interstellar grains. Based on an assumption that physico-chemical processes of S-bearing species on interstellar grains would be a key to constrain their presence in the ISM, several laboratory studies have been performed and our understanding has been significantly improved on the surface processes of S-bearing species at low temperatures[2,3]. In the present study, we further extend our understanding on the behavior of other S-bearing species, carbonyl sulfide (OCS) and methylmercaptan (CH_3SH), via non-energetic processes on interstellar ices at very low temperatures using experimental and computational methods.

We found that chemical reactions of OCS and H atoms proceeded via quantum tunneling, mainly resulting in the dissociation of the C-S bond: $OCS + H \rightarrow OCSH$, $OCSH + H \rightarrow H_2S + CO$. Further hydrogenation to the products leads to the formation of formaldehyde and methanol and the desorption of H_2S by chemical desorption. Another product of potential importance in astrochemistry would be thioformic acid (HCOSH), which was formed by successive H addition to OCS[4]. HCOSH has been recently detected toward the quiescent cloud G+0.693–0.027[5].

Similar to the case of OCS, the reaction of CH_3SH with H atoms was found to have multiple channels: $CH_3SH + H \rightarrow CH_3 + H_2S$, $CH_3S + H_2$, or $CH_2SH + H_2$. The major channel was the dissociation of C-S bond in CH_3SH with the activation barrier of 0.05 eV on amorphous solid water, eventually resulting in the formation of methane (CH_4) by further hydrogenation to CH_3[6]. 9The hydrogen abstraction channels lead to the formation of CH_3S and CH_2SH radicals, and further hydrogenation to these radicals would result in the formation of CH_3SH again. Chemical desorption of CH_3SH was not positively identified via these processes, implying the presence of other processes for the desorption of CH_3SH from interstellar grains at low temperatures.

1. V. Wakelam, A. Castets, C. Ceccarelli, et al. *A&A*, **2004**, 413, 60
2. A. Jiménez-Escobar, & G. M. Muñoz Caro, *A&A*, **2011**, 536, A91
3. Y. Oba, T. Tomaru, T. Lamberts, A. Kouchi, N. Watanabe, *Nat. Astron.* **2018**, 2, 228-232
4. T. Nguyen, Y. Oba, W. M. C. Sameera, A. Kouchi, N. Watanabe, *ApJ*, **2021**, 922, 146
5. L. F. Rodríguez-Almeida, I. Jiménez-Serra, V. M. Rivilla, et al. ApJL, **2021**, 912, L11
6. T. Nguyen, Y. Oba, W. M. C. Sameera, K. Furuya, A. Kouchi, N. Watanabe, *ApJ*, **2023**, in press.

Dissociative charge exchange processes between He^+ and CH_3CN and CH_3OH: a computational study

Noelia Faginas-Lago[1,2], Emília Valença Ferreira de Aragão[2], Luca Mancini[1], Marzio Rosi[3], Fernando Pirani[1,3] and Daniela Ascenzi[4]

[1]Dipartimento di Chimica, Biologia e Biotecnologie, Università degli studi di Perugia, via Elce di Sotto 8, 06123 Perugia, Italy

[2]Master-TEC s.r.l., Via Sicilia 41, 06128 Perugia, Italy

[3]Dipartimento di Ingegneria Civile ed Ambientale, Università degli studi di Perugia, Via G. Duranti 93, 06125 Perugia – Italy

[4]Department of Physics, University of Trento, Via Sommarive 14, 38123 Povo, Trento – Italy

e-mail: noelia.faginaslago@unipg.it

According to the Cologne Database for Molecular Spectroscopy website, as of February 2023 "about 290 molecules have been detected in the interstellar medium"[1]. In order to develop astrochemical models that match observed abundances, it is crucial to improve current chemical networks by including reliable rate constants for the production and destruction of interstellar Complex Organic Molecules (iCOMs). Helium, the second most abundant element in the Universe, can be ionized by cosmic rays to generate $He^{\bullet+}$. Due to the larger ionization energy of He with respect to organic molecules, collisions of iCOMs with $He^{\bullet+}$ leads to the decomposition of the molecules, as demonstrated in previous works on CH_3OCH_3 [2,3], $HCOOCH_3$ [2,4] and CH_3OH [5].

In this work, the results of a computational study on the reactions of destruction of two detected iCOMs, methanol (CH_3OH) and acetonitrile (CH_3CN), by collision with $He^{\bullet+}$ is presented. The dissociative charge (electron) exchange mechanism has been obtained by computing the entrance and exit multidimensional Potential Energy Surfaces (PESs). For the reaction between methanol and $He^{\bullet+}$, the non-adiabatic transitions between the PESs have been modeled using an improved Landau-Zener-Stückelberg approach[2-5]. For the reaction between acetonitrile and $He^{\bullet+}$, preliminary results of the investigation are presented.

1. H. S. P. Müller, S. Thorwirth, D. A. Roth, G. Winnewisser, *Astron. Astrophys.* **2001**, 370(3), L49–L52. Website: https://cdms.astro.uni- koeln.de/classic/molecules, last accessed on 27 February 2023.
2. D. Ascenzi, A. Cernuto et al., *Astron. Astrophys.* **2019**, 625, A72.
3. A. Cernuto, P. Tosi et al., *Phys. Chem. Chem. Phys.* **2017**, 19, 19554–19565.
4. A. Cernuto, F. Pirani et al. *ChemPhysChem.* **2018**, 19, 51-59.
5. V. Richardson, E. Valença Ferreira de Aragão et al., *Phys. Chem. Chem. Phys.* **2022**, 24, 22437-2245.

Experimental Study of the Binding Energy of NH_3 on Different Types of Ice

S. Kakkenpara Suresh[1,2], F. Dulieu[2], and J. Vitorino[2]

[1]*Max Planck Institute for Extraterrestrial Physics, Giessenbachstrasse 1, Garching 85748– GERMANY*

[2] *Laboratoire d'etudes du Rayonnement et de la Matiere en Astrophysique et Atmospheres, CY Cergy Paris Université, 5 Mail Gay Lussac, Cergy 95000 – FRANCE*

e-mail: shreyaks@mpe.mpg.de

N-bearing molecules (like N_2H^+or NH_3) are excellent tracers of high-density and low-temperature regions, such as dense cloud cores. Moreover, they could shed light in understanding snowlines in protoplanetary disks and the chemical evolution of comets. However, a lot remains unknown about the chemistry of these N-bearing molecules on grain surfaces - which could play an important role in their formation and evolution.

In this work, we experimentally study the behaviour of NH_3 on surfaces that mimic grain surfaces under interstellar conditions in the presence of some of the other major components of interstellar ices (i.e. H_2O, CO_2, CO). We measure the binding energy distributions of NH_3 from different H_2O ice substrates. We performed laboratory experiments using the Ultra High Vacuum (UHV) setup VENUS (VErs des NoUvelles Syntheses), where we co-deposited NH_3 along with other adsorbates (here H_2O, CO_2, CO) and performed Temperature Programmed Desorption (TPD) experiments. The experiments were monitored using a Quadrupole Mass Spectrometer (QMS). We obtained the binding energy of NH_3 on Crystalline Ice (CI) and compact-Amorphous Solid Water ice (c-ASW) by analysing the TPD profiles of NH_3 obtained after consequent depositions on these substrates.

In the co-deposition experiments, we observe a significant delay in the desorption and a decrease of the desorption rate of NH_3 when H_2O is introduced into the co-deposited mixture of NH_3-^{13}CO or NH_3-CO_2, which isn't the case in the absence of H_2O. Secondly, we notice that H_2O traps roughly 5-9% of the co-deposited $NH_{3,}$ which is released during the phase change of water from amorphous to crystalline. Thirdly, we obtain a distribution of binding energy values of NH_3 on both the ice substrates instead of an individual value as assumed in previous works. For CI, we obtained an energy distribution between 3780K - 4080K, and in the case of amorphous ice, the binding energy values are distributed between 3630K - 5280K - in both cases using a pre-exponential factor of $A = 1.94x10^{15}s^{-1}$.

From our experiments, we conclude that the behaviour of NH_3 is significantly influenced by the presence of water owing to the formation of hydrogen bonds with water, in line with quantum calculations. This interaction, in turn, preserves NH_3 on the grain surfaces longer and to higher temperatures making it available closer to the central protostar in protoplanetary disks than previously thought. It explains well why NH_3 freeze out in prestellar cores is efficient. This may impact the overall composition of comets, particularly the desorption of molecules from their surface as it approaches the Sun.

Formation of Insoluble Organic Material from Meteoritic Organic Analogs

Michel Nuevo[1], Brian C. Ferrari[2,3], Scott A. Sandford[1], Christopher J. Bennett[2],
Yu-Jung Chen[4], and Yu-Jong Wu[5]

[1]*NASA Ames Research Center, Space Science and Astrobiology, Moffett Field, CA – USA*
[2]*University of Central Florida, Astrochemistry Laboratory, Orlando, FL – USA*
[3]*Leiden University, Institute of Chemistry, Leiden – The Netherlands*
[4]*National Central University, Department of Physics, Taoyuan – Taiwan*
[5]*National Synchrotron Radiation Research Center, Hsinchu – Taiwan*
e-mail: michel.nuevo@nasa.gov

We present preliminary results from the study of several mixtures of analogs of organics found in meteorites that were exposed to ultraviolet (UV)/extreme UV (EUV) photon radiation to study the evolution of their chemical and elemental compositions as a function of the radiation dose. These experiments aim at simulating the high radiation doses experienced by organic materials coating grains in the protosolar nebula[1]. The mixtures of organics were prepared by mixing commercial standards of soluble compounds found in meteorites in HPLC-grade water, including: amino acids (both found and not found in terrestrial life), nucleobases (building blocks of DNA/RNA) and derivatives, and sugar derivatives (sugars, sugar alcohols, sugar acids, both found and not found in terrestrial life). The proportions between the components of the different mixtures were chosen either to simulate their relative proportions in meteorites or to be used as a model to be compared against. Some mixtures only included compounds of the same family, i.e., amino acids or nucleobases or sugar derivatives, while other mixtures included compounds of two or three families of compounds. Each mixture was dried under vacuum, re-dissolved with HPLC-grade methanol, and dried on 6 spots on a pre-baked (500 °C) aluminum foil strip by depositing small aliquots (~50 µL) and letting the methanol evaporate. The resulting sample were analyzed with infrared (IR) microscopy.

The samples where and then exposed to UV/EUV photons at a synchrotron facility, on a beamline providing a broad-band photon beam in the 4–45-eV range with a ~10^{16} photons s^{-1} flux[2]. Each sample was exposed to increasing UV/EUV radiation doses ranging from ~10^{18} to ~10^{21} photons, i.e., covering 4 orders of magnitude. After UV/EUV irradiation, all the irradiated samples were analyzed with IR microscopy, and the data compared to those before irradiation to identify changes in chemical composition as a function of the photon dose. UV/EUV-irradiated residues are also expected to be analyzed with other techniques including X-ray absorption spectroscopy (XAS) and AROMA (high-resolution spectroscopy). Results will be compared with data from extraterrestrial materials such as meteoritic insoluble organic material (IOM).

1. F.J. Ciesla, S.A. Sandford, *Science* **2012**, 336, 452-454
2. M. Nuevo, Y.-J. Chen, W.-J. Hu, et al., *Astrobiology* **2014**, 14, 119-131

Gas-phase formation route of glycine in the interstellar medium

Nadia Balucani[1], Andrea Giustini[1], Cecilia Ceccarelli[2], Marzio Rosi[3], and Massimiliano Aschi[4]

[1]*Università degli Studi di Perugia, Dipartimento di Chimica, Biologia e Biotecnologie, 06123 Perugia – Italy*

[2] *Université Grenoble Alpes, CNRS, IPAG, 38000 Grenoble, France*

[3]*Università degli Studi di Perugia, Dipartimento di Ingegneria Civile e Ambientale, 06127Perugia, Italy*

[4]*Università degli Studi dell'Aquila, Dipartimento di Scienze Fisiche e Chimiche, 67010 L'Aquila– Italy*

e-mail: nadia.balucani@unipg.it

Having the formula NH_2-CH_2-COOH, glycine (Gly) is the simplest stable amino acid. Its simplicity suggests that it might be formed in abiotic processes of the kind we see in action also in extreme extraterrestrial environments like those typical of the interstellar medium where even more complex organic molecules have been observed [1]. In spite of its simplicity, however, Gly is one of the 20 genetically encoded (proteinogenic) amino acids that are fundamental for life as we know it and its formation route in primitive Earth is a subject of great interest in prebiotic chemistry [2].

After its tentative detection [3] in 2003 (not confirmed by other attempts [4,5]), the possible formation routes of Gly have been widely investigated. A recent review has summarized all the available experimental and theoretical investigations that have tried to identify possible Gly formation routes (see Rimola et al. [2]). However, none of them seems to be a convincing candidate for interstellar Gly formation.

In this contribution, a chemical scheme leading to glycine formation in the gas-phase is proposed. It is based on an analogy with the chemistry leading from ethanol to its daughter species [6]. Dedicated electronic structure calculations have been performed to test the validity of the chemical scheme proposed and the derived rate coefficients have been employed in simple astrochemical model to verify whether glycine can reach an abundance high enough to allow its detection. Encouraging results have been obtained.

1 C. Ceccarelli et al., in Protostars & Planets VII, 2023, https://doi.org/10.48550/arXiv.2206.13270

2 A. Rimola, N. Balucani, C. Ceccarelli, P. Ugliengo, *Int. J. Mol. Sci*. **2022**, 23, 4252

3 Yi-Jehng Kuan *et al*., *Astrophys. J.* **2003**, 593, 848

4 C. Ceccarelli et al., *Astron. Astrophys*. **2000**, 362, 1122

5 L. E. Snyder et al., *Astrophys. J.* **2005**, 619, 914

6 D. Skouteris et al., *Astrophys. J.* **2018**, 854,135

How The Formation Of Water In Presence Of Other Molecules Influences The Chemistry Of Dust Grains

B. Husquinet[1,2], J. Vitorino[1], P. Casseli[2], and F. Dulieu[1]

[1]*CY Cergy Paris Université, Observatoire de Paris, PSL Université, Sorbonne Université, CNRS, LERMA, 95000 Cergy, France*

[2] *Max-Planck-Institut für extraterrestrische Physik, Gießenbachstraße 1, Garching, 85748, Germany*

e-mail: basile.husquinet@cyu.fr

In the dense region (>10^4 cm^{-3}) and at low temperature (<12K) as in the pre-stellar core, the molecules are totally adsorbed by the dust grains[1]. However, observations show an unexplained number of molecules in the gas phase[2] while this region is isolated from UV and CR. The most efficient type of desorption in this environment is chemical desorption[3,4]. Even complex molecules (iCOM) like methanol desorb[5].

For this poster, we will differentiate two types of chemical desorption, direct and indirect chemical desorption (see figure 1). At the left panel, the excess energy due to the chemical reaction makes the newly created molecule desorb (direct mode). At the right panel, the excess of energy due to the chemical reaction is transmitted to a neighboring molecule which has made it desorb (indirect mode). We will show experimental results of indirect chemical desorption focusing on the OH+H->H2O reaction which is very energetic. For this, we codeposit O2 and H to form the water molecule with a third molecule X which is not very reactive (i.e N2, CO...). The measured amount of molecule X is lower when we codeposit with O2+H than we deposit only the molecule X.

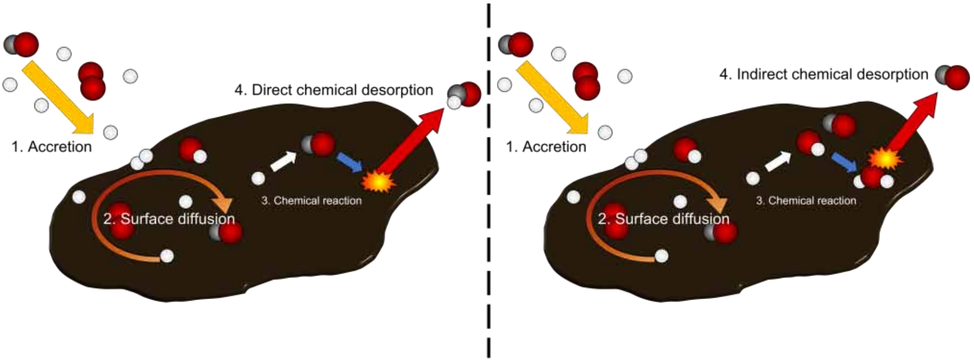


Figure 1: *Sketch of the direct chemical desorption à the left panel and the indirect chemical desorption at the right panel.*

1. M. P. Collings, M. A. Anderson, R. Chen, et al. , *MNRAS*, **2004**, 354, 1133
2. A. Bacmann, V. Taquet, A. Faure, C. Kahane, C. Ceccareli, *A&A*, **2012**, 541, L12
3. F., Dulieu, E. Congiu, J. Noble, et al., *Scientific Reports*, **2013,** 3, 1338
4. M. Minissale, F. Dulieu, S. Cazaux, S. Hocuk, *A&A*, **2016**, 585, A24
5. M. Minissale, A. Moudens, S. Baouche, H. Chaabouni, F. Dulieu, *MNRAS*, **2016,** 458, 2953

In Situ Experimental Study Of Photo-conversion Rates Of Ices In Protoplanetary disks

C. Assadourian[1], F. Borget[2], C. Laffon[1], Ph. Parent[1]

[1] *University of Aix Marseille, CNRS, CINaM, Marseille, France*

[2] *University of Aix Marseille, CNRS, PIIM, Marseille, France*

e-mail : celine.assadourian@univ-amu.fr

Around the young stars of solar type T Tauri, the ices at the origin of the formation of planetesimals in protoplanetary disks undergo strong UV and X radiation. These ices migrate over several AUs due to the disk evolution in $\sim 10^6$ years, the trajectory simulated by Ciesla at al.[1] shows that UV represent only 5% of the total radiation undergone by ices. By extrapolation, the typical X-ray dosage for these ices is 95%. X-rays, between 0.1 to 10keV, emitted in abundance penetrate deeper into the disk, and significantly affect the chemistry of the ices[2]. In the literature, it's mainly the effects of UV radiation on ice that have been studied[3-5]. Here, we want to study the impact of X-radiations on the evolution of ice and compare them to UV.

In laboratory we synthesize different ices species present at the surface of the grain (H_2O, CH_3OH, CO_2, HCN)[6] in UHV cryogenic chamber SUMO at the CINaM laboratory. Ices are grown on a gold plate by controlling the pressure of chemical species in the chamber with mass spectroscopy (QMS) and gauge pressure. The experimental set-up is equipped of a 1.4 keV X-ray source, and a microwave-discharged UV hydrogen flow lamp to simulate the radiation in the disk. We use X-ray photoelectron spectroscopy (XPS) and FTIR spectroscopy in reflection mode (FT-RAIRS), to follow and characterize the photochemical evolution of our ices. Our research will complement and enrich previous work in synchrotron X-ray radiation[7-8]. We have developed an analytical method to extract X-ray photo-conversion rates, and to compare them to UV photo-conversion rates. In this sense, we can obtain the photolysis cross sections and photodesorption yields of methanol, carbon dioxide or hydrogen cyanide ice mixed with water.

1 F. J. Ciesla, S. A. Sandford, *Science*, **2012,** 336, 452

2 C. Walsh, H. Nomura, T.J. Millar, Y. Aikawa, *Astrophys. J.*, **2012,** 747

3 P. Theule, F. Borget, F. Mispelaer, G. Danger, F. Duvernay, J. C. Guillemin, T. Chiavassa, *Astronomy & Astrophysics*, **2011**, 534

4 P.A. Gerakines, W.A. Schutte, and P. Ehrenfreund, *Astronomy & Astrophysics*, **1996**, 312, 289-305

5 F. Borget, S. Müller, D. Grote, P. Theulé, V. Vinogradoff, T. Chiavassa, W.Sander, *Astronomy & Astrophysics*, **2017**, 598

6 E.L. Gibb, D.C.B. Whittet, A.C.A. Boogert, A.G.G.M. Tielens, *The Astrophysical Journal Supplement Series*, **2004**, 151:35

7 C. Laffon, S. Lacombe, F. Bournel, P. Parent, *J. Chem. Phys*., **2006**, 125

8 R. Dupuy, M. Bertin, G. Féraud, M. Hassenfratz, X. Michaut, T. Putaud, L. Philippe, P. Jeseck, M. Angelucci, R. Cimino, V. Baglin, C. Romanzin, J.H. Fillion, *Nat. Astron. 2,* **2018**, 796–801

New Chemistry on Rotating Grain Surfaces: Rotational and Rotational-thermal Desorption Mechanisms

Le Ngoc Tram[1] and Thiem Hoang[2]

[1]*Max-Planck institute for Radio Astronomy, Auf dem Hügel 69, Bonn 53121 – GERMANY*

[2] *Korea Astronomy and Space Science Institute, Daejeon 34055 – KOREA*

e-mail: nle @mpifr-bonn.mpg.de

Interstellar complex organic molecules (iCOMs) are thought to form on the surface of grains and subsequently returned into the gas due through the desorption process. Previous research on the desorption of molecules from the ice mantle assumed that grains are at rest, which is contrary to the fact that grains are suprathermally rotating as a result of their interaction with an anisotropic radiation or gas flow. We[1] demonstrated that when the radiation field intensity is sufficient, suprathermal rotating grain could break up the thick ice mantle into small fragments by centrifugal stress. Consequently, we found that tiny fragments exhibit a transient release of COMs due to thermal spikes, whereas larger fragments can facilitate thermal sublimation at much higher rates than from the original icy grain. We named this new mechanism as *rotational desorption*. Furthermore, we[2] introduced that the centrifugal energy induced on a thinner icy mantle reduces the potential barrier and enhances the desorption rate. This non-thermal process is called *rotational-thermal desorption*. We found that this desorption is much more efficient than thermal desorption for molecules with high binding energy such as water and COMs. Our new mechanisms have important implications for understanding the origin of COMs detected in star-forming regions and call for attention to the effect of suprathermal rotation of icy grains to use molecules as a tracer of physical conditions in such conditions.

1. T. Hoang & L.N. Tram, *ApJ*. **2020**, 891:38
2. T. Hoang & N.D. Tung, *ApJ*, **2019**, 885:125

NH_4SH Formation And Behavior On Interstellar Dust Grain Analogues

J. Vitorino[1], J.-C. Loison[2], E. Congiu[1], and F. Dulieu[1]

[1]*CY Cergy Paris Université, Observatoire de Paris, PSL University, CNRS, LERMA, 5 Mail Gay-Lussac, F-95000, Neuville-sur-Oise, France*

[2]*Université de Bordeaux, Institut des Sciences Moléculaires, 351 Cours de la Libération, F-33405, Talence, FRANCE*

e-mail: julie.vitorino@cyu.fr

In comets and in the cold phase of the interstellar medium (ISM), salts – especially ammonium salts – are considered to be highly important molecular species due to their properties. The interactions between the cation and anion involved in the salt bond are strong enough to allow both species to remain on dust grains in the form of salt, far beyond their respective desorption temperatures as pure species[1]. This would partly explain the nitrogen depletion observed in various environments[2,3], compared to the Solar System ratios[4]. In the case of sulfur, the H_2S/OCS ratio observed in protostars could be explained by the presence of ammonium hydrosulfide (NH_4SH) salts[5].

Laboratory data about NH_4SH characteristics in ISM cold relevant conditions are rather scarce[6]. We propose to densify the laboratory data regarding the formation, signatures, characteristics, desorption, and hydrogenation behavior of NH_4SH on interstellar dust grain analogues.

Temperature programmed desorption experiments and Fourier transform infrared reflection spectroscopy were performed at high and low temperatures, on a gold surface, with and without a water ice matrix, to monitor the behavior of NH_4SH.

The salt is found to form in situ at 10K, from a mixture of ammonia (NH_3) and hydrogen sulfide (H_2S). The NH_4^+ infrared feature is the most prominent at 80K. As pure species, H_2S and NH_3 desorb at 76K and 90K, respectively. When in the form of salt, they are released at 153K into the gas phase. The presence of water delays the desorption of the salt until the very end of the water desorption, but does not influence the desorption kinetics. Additionally, we showed that excessive NH_3 is solvated in the final mixture. Finally, NH_4SH reacts efficiently with H, most likely producing H_2S and solvated ammonia.

1. F. Kruczkiewicz, J. Vitorino, E. Congiu, P. Theulé, F. Dulieu, *A&A*. **2021**, 652, A29

2. G. Filacchione, O. Groussin, C. Herny, *Space Sci. Rev.* **2019**, 215, 19

3. B. D. Savage, K. R. Sembach, *ARA&A*. **1996**, 34, 279

4. K. Lodders, in Principles and Perspectives in Cosmochemistry, Springer Berlin Heidelberg, **2010**, 379-417

5. T. Kushwahaa, M. N. Drozdovskaya, L. Tychoniec, B. Tabone, *A&A*. **2023**, arXiv preprint, arXiv:2302.09452

6. M. J. Loeffler, R. L. Hudson, N. J. Chanover, A. A. Simon, *Icarus*. **2015**, 258, 181-191

Non-thermal desorption of complex organic molecules in protoplanetary disks: a computational study

Aneesa Ahmad[1] and Catherine Walsh[1]

[1]*University of Leeds, Department of Physics and Astronomy, Sir William Henry Bragg building, Woodhouse, Leeds – United Kingdom*

[2] *School of Physics and Astronomy, Sir William Henry Bragg building, University of Leeds, Woodhouse, Leeds – United Kingdom*

e-mail: a.ahmad@leeds.ac.uk

Stars and their surrounding planetary systems form within dense molecular clouds. During the gravitational collapse of these clouds, dust and gas flows through a collapsing envelope, feeding a so-called protoplanetary disk, providing the material required to form a new planetary system.[1]

The cold midplane of protoplanetary disks is seeded with ices that originally formed on dust grains at the low densities (10^3 – 10^4 cm^{-3}) and temperatures (10 K) in the parent molecular cloud.[2] Infrared observations of molecular clouds have well-characterised the composition of these ices. They are mainly composed of simple hydrogenated species such as H_2O, CH_4, and NH_3, with CO and CO_2 ices also forming when the temperature is low enough for CO to freeze out (< 20 K). CO-rich ices can subsequently react with atomic hydrogen to form larger and more complex species such as H_2CO and CH_3OH, the processing of which via heat and/or radiation can further enhance the chemical complexity of interstellar ices.[4]

The presence of complex organic molecules (in the form of gas-phase methanol) in protoplanetary disks have finally been revealed around solar-type stars in observations with ALMA (the Atacama Large Millimeter/submillimeter Array);[5] the methanol is found to be rotationally cold and likely arising from non-thermal desorption from the cold icy reservoir in the disk midplane.[6] In this work we have carried out theoretical modelling of the non-thermal desorption of complex organic molecules in water-rich ices by stellar UV radiation. Our aims are to predict the desorption outcomes and yields for ices irradiated by a range of radiation fields suitable for young stars and for the different ice environments expected in planet-forming disks. In this poster, we explain the motivation behind this work, and show the results of some preliminary simulations. This research has been carried out using molecular dynamics simulations performed using the GROMACS software package.

[1] Ewine F. van Dishoeck and Edwin A. Bergin. "Astrochemistry associated with planet formation." *arXiv preprint arXiv:2012.01472* (2020)
[2] Jes K. Jørgensen, Arnaud Belloche, and Robin T. Garrod. "Astrochemistry during the formation of stars." *Annual Review of Astronomy and Astrophysics* **58** (2020): 727-778.
[3] Boogert, A. C. A., Gerakines, P. A., and Whittet, D. C. B. "Observations of the Icy Universe." *Annual Review of Astronomy and Astrophysics* **53** (2015): 541-581.

Rearrangement Pathways to form Cyano-indene, an Interstellar PAH, and its Photoelectron Spectroscopic Characterization

Mayank Saraswat[1], Adrian Portela-Gonzalez[1], Enrique Mendez-Vega[1], Ginny Karir[1],
Patrick Hemberger*[2], and Prof. Wolfram Sander*[1]
[1]Lehrstuhl für Organische Chemie II, Ruhr- Universität Bochum, 44780 Bochum, Germany
[2]Laboratory for Synchrotron Radiation and Femtochemistry, Paul Scherrer Institut, CH-5232 Villigen, Switzerland
e-mail: Mayank.saraswat@ruhr-uni-bochum.de

The presence of polyaromatic hydrocarbons (PAHs) in the interstellar medium has been postulated since the late 1980s based on the diffuse infrared emission bands detected.[1] Deciphering individual PAHs, however, has remained difficult with the first individual detection for a PAH, indene, only coming in 2022 (McGuire et al and Cernicharo et al.).[2a,b] In the past 5 years, multiple breakthrough discoveries of smaller cyclic and aromatic (or non-aromatic) molecules (especially N-substituted rings) in interstellar medium (ISM) has set up for a very exciting time as we start to understand the PAH chemistry in space.

Usually, two approaches- top-down and bottom-up are considered for the formation of PAHs in the ISM. Heterocyclic PAHs, especially nitrogen substituted, are also postulated to contribute to certain diffuse bands detected, however, no nitrogen-substituted aromatic ring has been detected so far. Given the detection of cyanide-substituted aromatic rings/PAHs, the presence of isomerized species within the same molecular formula (eg. $C_XH_YN_Z$) cannot be ruled out, especially in environments with high temperatures. Some of the detected isomeric species are (a) C_9H_7N: 2-cyano indene (b) C_6H_5N: 1-cyano-cyclopentadiene and 2-cyano-cyclopentadiene; (c) $C_{11}H_7N$: 1-cyanonaphthalene and 2-cyanonaphthalene; (d) C_5H_3N: vinylcyanoacetylene and cyanovinylacetylene.[3] This highlights a very rich chemistry in these interstellar environments, including PAHs and potentially their nitrogen-containing analogues (PANHs). Exploring the reactions forming these species and other isomeric PAHs is thus crucial.

In this work, we investigated and characterized cyano-indene isomers from the thermal rearrangement of 2-naphthylnitrene using FVP of naphthylazide coupled with VUV irradiation. Three isomeric cyano-indenes have been characterized using photoion mass-selected threshold photoelectron spectroscopy (ms-TPE) and deduced the mechanism of formation of these thermal rearrangement products from 2-naphthylnitrene. Accurate adiabatic ionization energies of cyano-indenes were determined experimentally from ms-TPE and also fitted with Franck−Condon (FC) simulations.

1. C. Joblin, A. Tielens, V. Bierbaum, V. LePage, T. Snow, *EAS Publications Series*. **2011**, 46, 427-440
2. (a) J. Cernicharo, M. Agundez, C. Cabezas, B. Tercero, N. Marcelino, J. R. Pardo, P. de Vicente, *A&A* **2021**, 649, L15; (b) A. M. Burkhardt, K. L. K. Lee, P. B. Changala, C. N. Shingledecker, I. R. Cooke, R. A. Loomis, H. Wei, S. B. Charnley, E. Herbst, M. C. McCarthy, et al. *ApJL* **2021**, 913, L18
3. K. L. K. Lee, R. A. Loomis, A. M. Burkhardt, I. R. Cooke, C. Xue, M. A. Siebert, C. N. Shingledecker, A. Remijan, S. B. Charnley, M. C. McCarthy, *ApJL* **2021**, 913, L11

Rivers in The Sky: Streamers Toward Two Embedded Sources in Perseus

M. T. Valdivia-Mena[1] , J. E. Pineda[1], D. M. Segura-Cox[2], and P. Caselli[1]

[1]*Max-Planck-Institut für extraterrestrische Physik, Giessenbachstrasse 1, D-85748 Garching — GERMANY*

[2] *Department of Astronomy, The University of Texas at Austin, 2515 Speedway, Austin, TX 78712 – USA*

e-mail: mvaldivi@mpe.mpg.de

In the last few years, there has been a rising number of streamers discovered[1,2,3]. Streamers are long gas structures (~ 1000-10000 au) that feed material to protostellar systems from both within and outside their natal cores[4]. This newly observed infall mechanism can replenish the protostellar disk with chemically fresh material, rejuvenating the gas available to form planets.

I present streamers found toward two embedded protostars in Perseus; both are still surrounded by some material from their natal core but were previously thought to be beyond their accretion phase. Per-emb-50 is located in the middle of the active star forming region NGC 1333. We found that its streamer delivers mass with a rate 5 to 10 times larger than the accretion rate from disk to protostar, implying an accumulation of mass within the disk that may trigger gravitational instabilities or accretion outbursts[3]. The second streamer was identified toward B5-IRS1, an isolated protostar in the Barnard 5 dense core. Using a clustering algorithm, we disentangled the streamer from the rest of the envelope emission and determined that it deposits material on disk scales (~250 au).

Our results suggest that both streamers originate from close-by fibers, kinematic substructures of the extremely large-scale filaments that harbor protostellar cores. These two streamers show that the local environment around protostars influences disk evolution even after the traditional main accretion phase.

1. J. E. Pineda, D. M. Segura-Cox, P. Caselli, et al., *Nature Astronomy* **2020**, 4, 1158
2. A. Garufi, L. Podio, C. Codella, et al., *A&A* **2022**, 658, A104
3. M. T. Valdivia-Mena, J. E. Pineda, D. M. Segura-Cox, et al., *A&A* **2022**, 667, A12
4. J. E. Pineda, D. Arzoumanian, Ph. André, et al., *Protostars and Planets VII* **2023**

S(^{1}D) insertion reactions on the surface of ice mantles. An overlooked mechanism to form S-containing organic species?

Gabriella Di Genova[1], Nadia Balucani,[1] Andrea Giustini[1], Cecilia Ceccarelli[2], Marzio Rosi[3]

[1]*Università degli Studi di Perugia, Dipartimento di Chimica, Biologia e Biotecnologie, 06123 Perugia – Italy*

[2] *Université Grenoble Alpes, CNRS, IPAG, 38000 Grenoble, France*

[3]*Università degli Studi di Perugia, Dipartimento di Ingegneria Civile e Ambientale, 06127Perugia, Italy*

e-mail: gabriella.digenova@studenti.unipg.it

The chemistry leading to interstellar sulphur-bearing organic molecules is still in need to be fully characterized. Sulphur is present in space with an abundance of 16 ppm and it is an interesting element for prebiotic chemistry since it is present in amino acids and several other biomolecules. Simple S-containing species, such as OCS, CS, CH_3SH, H_2CS, as well as C_2S and C_3S, have been detected in a variety of objects [1]. More complex sulphur species have been detected in the coma of the comet 67P/Churyumov-Grasimenko [2], such as CH_4OS, C_2H_6OS, C_3H_6OS and CH_4S_2.

In this contribution, we present a theoretical investigation of two reactions involving atomic sulphur in its first electronically excited state, ^{1}D, with two molecules, water and methanol, which are abundant in interstellar/cometary ice. S(^{1}D) can be produced on the ice surface by UV-induced photodissociation of precursor molecules, such as OCS, that is, one the few molecules for which a secure identification in interstellar ice has been provided [3]. The ^{1}D state is metastable with a long radiative lifetime and is very reactive, differently from the case of the ground ^{3}P state of atomic sulphur.

The role of electronically excited metastable atoms in the ice chemistry has been recently considered in the research groups of Oberg and Herbst [4,5] for the similar case of atomic oxygen (which is also characterized by a ground ^{3}P and an excited ^{1}D state). According to those studies, the formation of O(^{1}D) opens up new reaction pathways which are not amenable in the case of the O(^{3}P) reactions. Previous work from our laboratory has focused on the reactions of S(^{1}D) atoms with saturated and unsaturated hydrocarbons [6,7] confirming that S(^{1}D) can lead to the formation of molecules holding a novel C-S bond. In this work we have shown that species like CH_2OHSH (mercaptomethanol) are efficiently formed.

This project has received funding from the Italian MUR (PRIN 2020 "Astrochemistry beyond the second period elements", Prot. 2020AFB3FX) and the Italian Space Agency (Life in Space project ASI N. 2019-3-U.0).

1 See, for instance, V. Taquet et al., *Astron. Astrophys*. **2020**, 637, A63.

2 N. Hänni et al., *Nat. Commun*. **2022**, 3639, 13

3 A. C. A. Boogert et al., *Astrophys. J*. **2022**, 941, 32

4 J. B. Bergner et al., *Astrophys. J*. **2019**, 874,11

5 J. T. Carder et al., *MNRAS* **2021**, 508, 1526

6 F. Leonori et al., *PCCP* **2009**, 11, 4701; *J. Phys. Chem. A 2009*, 113, 4330

Spectroscopy of Small Phosphorus-Containing Molecules of Astrophysical Interest

Elavenil Ganesan[1], Arun-Libertsen Lawzer[1], Thomas Custer[1], Jean-Claude Guillemin[2], and Robert Kołos[1],

[1]*Institute of Physical Chemistry, Polish Academy of Sciences, 44 Kasprzaka St., PL-01-224, Warsaw, POLAND*

[2]*University of Rennes, Ecole Nationale Superieure de Chimie de Rennes, CNRS-IRCR, 6226,*
F-35000, Rennes, FRANCE

e-mail: eganesan@ichf.edu.pl.

Only several phosphorus-containing species, namely PN, PO, CP, CCP, HCP, SiP, PO^+, PH_3,[1] (and perhaps NCCP) already belong to the inventory of ca. 300 currently known inter- and circumstellar molecules. More will certainly be found. But the available spectroscopic information on many small, potentially astrochemical P-bearing compounds is scarce (often limited to microwave transitions). Our Warsaw group is trying to bridge that gap with the missing vibrational and electronic spectroscopy data.

This contribution will provide our recent results on several products photochemically obtained from certain precursor compounds – namely phosphaethyne (HCP), methylphosphine (CH_3-PH_2), phosphapropyne (CH_3-CP), and bisphosphinomethane (PH_2-CH_2-PH_2) – subjected to UV radiation. The most important photodehydrogenation products were $H_2C{=}PH$ (we provided the vibrational frequencies), CP (phosphorescence)[2], HCCP (IR and UV absorption spectra)[3], and PCP (optical absorption). We investigate these species, highly unstable at standard laboratory conditions, using the environment of cryogenic noble-gas solids (“matrices”). Spectral assignments are assisted with quantum chemical predictions.

1. V. M. Rivilla, J. G. D. L. Concepción, I. Jiménez-Serra , J Martín-Pintado, L. Colzi, B. Tercero, A. Megías, Á. López-Gallifa, A. Martínez-Henares, S. Massalkhi, S. Martín, S. Zeng, P. D. Vicente, F. Rico-Villas, M. A. R. Torres and G. Cosentino, *Front. Astron. Space Sci.* **2022**, 9, 829288.
2. E. Ganesan, T. Custer, A.-L. Lawzer, J. -C. Guillemin, & R. Kołos, *Angew. Chem. Int. Ed.* **2022,** 61, 43.
3. A.-L. Lawzer, T. Custer, J. -C. Guillemin, & R. Kołos, *Angew. Chem. Int. Ed*, **2021,** 60, 12, 6400–6402.

The Chemical Composition Of A Protostellar Envelope With Luminosity Outbursts

Pierre Marchand[1] , Audrey Coutens[1], and Jules Scigliuto[2]

[1]*Insitut de Recherhe en Astrophysique et Planétologie, 9 avenue du Colonel Roche, 31400 Toulouse, France*

e-mail: pierre.marchand@irap.omp.eu

Accretion variability in protostars can lead to luminosity outbursts that heat up protostellar envelopes. This rise in temperature pushes back the snowlines, releasing in the gas phase molecules previously frozen on dust grains, which affects the whole chemical dynamics. In this work, we seek to observe the impact of this mechanism on the chemical composition of the protosellar envelope. We present a IRAM-30m spectral survey of a protostar that underwent such a luminosity outburst, and compare it to quiescent protostars. We obsserve in particular the presence of many carbon chains.

The Impact Of Luminosity Bursts On The Chemistry Of Protostars

Antoine Espagnet[1] , Audrey Coutens[1], and Pierre Marchand[1]

[1] *Institut de Recherche en Astrophysique et Planétologie (IRAP), Université de Toulouse, UPS-OMP, CNRS, CNES, 9 av. du Colonel Roche, F-31028 Toulouse Cedex 4, France*

e-mail: antoine.espagnet@irap.omp.eu

Characterizing the diversity of chemical compositions of solar-type protostars is essential to understand the conditions in which our Sun formed. Some YSO (Young Stellar Objects) are known to experience luminosity bursts[1] during their evolution during both protostellar phase (Class 0-I) and pre-main sequence phase (Class II). Such events are due to a significant increase of the mass accretion rate[2]. The increase of luminosity leads to a warm up of the protostellar envelope. As temperature is a key parameter for gas-grain chemistry, we want to study the impact that the luminosity bursts can have on the chemistry of protostellar envelopes from the cold outer regions to the warm inner regions.

To understand how these bursts affect the chemistry of the envelope of the protostar we implemented the physical changes induced by luminosity bursts using numerical 1D simulations[3]. We then used the gas-grain chemistry code Nautilus to predict the abundances of molecules for luminosity outbursts with different characteristics. Finally we compared the results with the case without luminosity outburst to determine the impact of luminosity bursts on the chemistry.

1. Fischer, W. J., Hillenbrand, L. A., Herczeg, G. J., et al. 2022, Protostars and Planets VII, arXiv:2203.11257.

2. Audard, M., Ábrahám, P., Dunham, M. M., et al. 2014, Protostars and Planets VI, 387.

3. Vaytet, N. \& Haugbølle, T.\ 2017, \aap, 598, A116.

The S^+ + SiH_2 Reaction: Toward the Synthesis of Interstellar SiS

L. Mancini[1] , M. Rosi[2], D. Skouteris[3], F. Pirani[1], G. Di Genova[1], N. Balucani[1], C. Ceccarelli[4]

[1]*University of Perugia, Department of Chemistry, Biology and Biotechnology, via Elce di Sotto 8, Perugia –ITALY*

[2]*University of Perugia, Department of Civil and Environmental Engineering, via G. Duranti, Perugia –ITALY*

[3] *Master-tec s.r.l., via Sicilia 41, Perugia – ITALY*

[4]*Université Grenoble Alpes, IPAG, 38000 Grenoble-FRANCE*

e-mail: luca.mancini2@studenti.unipg.it

Silicon represents the seventh most abundant element in the universe and is mostly trapped in the dust grains present in the interstellar medium (ISM) in the form of silicates. Nevertheless, an increasing number of silicon-bearing molecules have been detected in different regions of the ISM, with a molecular size going up to 8 atoms. The presence of silicon in the gas phase is mainly related to violent events, such as shocks[1]. As soon as silicon is released in the gas phase, it can immediately react and it is mostly converted into SiO, which is considered a useful target to probe shock regions[1]. Another interesting Si-bearing molecule is silicon sulfide, SiS, detected for the first time in 1975[2] and more recently in a shocked region driven by a jet originated from a Sun-like protostar[1]. Interestingly, a surprisingly high abundance of SiS has been inferred in a well-localized region around the protostar, suggesting a different chemical origin for SiO and SiS. The reason for such a peculiar diversity is unknown and represents a challenge to our comprehension of interstellar silicon chemistry. Given the difficulties associated to the experimental investigation of the postulated reactions, theoretical quantum chemistry calculation appears to be pivotal to elucidate the chemistry of silicon-bearing species. Recently, some interesting analysis on the potential role of neutral gas-phase chemistry in the formation and destruction routes of SiS has been proposed, starting from neutral-neutral reactions (including SiH+S, SiH+S_2 and Si+HS[3-5]) suggesting a very important role for the SiS formation. Additionally, the effect of other reactions, including Si+SO_2, on the abundance of Si-bearing molecules, such as SiS and SiO, have been recently included in astrochemical models[6]. As a part of a systematic investigation on interstellar SiS formation, we have now focused on possible ion-molecules reactions. In particular, here we report on the theoretical characterization of the PES for the reaction between the S^+ cation and the SiH_2 radical, which can be formed by photodissociation or other high-energy processes involving SiH_4. Additionally, a proton transfer to neutral molecules with a large proton affinity like ammonia[7] is invoked for the formation of neutral SiS. The inclusion of the title reactions, together with other processes, in astrochemical models is currently under way.

1. L. Podio, C. Codella, B. Lefloch, N. Balucani, C. Ceccarelli et al., *MNRAS Lett.* **2017**, 470, L16–L20
2. A. Gusdorf, G.P. Des Forets, S. Cabrit, D. Flower, *A&A* **2008**, 490, 695–706
3. M. Rosi, L. Mancini, D. Skouteris, C. Ceccarelli, et al. *Chem. Phys. Lett.* **2018**, 695, 87–93
4. A. Zanchet, O. Roncero, M. Agundez, J. Cernicharo. *ApJ* **2018**, 862, 38
5. V. Mota, A. Varandas, E. Mendoza, V. Wakelam, B. Galvao. *ApJ* **2021**, 920, 37
6. D. R. Campanha, E. Mendoza M. Silva, V. Wakelam, B. Galvao et al. *MNRAS* **2022**, 515,369-377.
7. V. Taquet, E.S. Wirstrom, S.B. Charnley. *ApJ* **2016**, 821, 46

TABLE OF CONTENTS

Talks

22 **Dissipation of the Nascent Reaction Energy of Formamide Formation Route on Interstellar Water Ice Surfaces**
Berta Martínez-Bachs , Gerard Pareras, Joan-Enrique Romero and Albert Rimola

23 **The Role Of Low-Energy (< 20 eV) Electrons In Astrochemistry**
Christopher Arumainayagam, Qin Tong Wu, James Battat, and Marco Padovani

24 **Interstellar Ices Formation And Interaction With Molecules Of Astrochemical Interest: An *In Situ* Infrared Study**
Guillermo Escolano-Casado, Rosangela Santalucia, Lorenzo Mino, Giuseppe Spoto, and Piero Ugliengo

25 **Diffusion and sublimation of ices on comets and (icy)moons**
Stephanie Cazaux, Carla Tamai, Belen Mate, and Miguel Angel Satorre

26 **Laboratory constraints on thermal desorption of astrophysical ice analogues**
F. Kruczkiewicz, F. Dulieu, B. M. Giuliano, A. V. Ivlev, P. Caselli, C. Ceccarelli and P. Theulé

27 **Sticking Coefficients of Astrochemically-Relevant Ices on Realistic Grains Analogues are Lower than Expected**
Caroline Stadler, Daniel Ferry, Olivier Grauby, Philippe Parent, and Carine Laffon

28 **Unlocking the Interaction of the CN Radical with Interstellar Ices: An Atomistic View of Polar and Apolar Environments**
Joan Enrique-Romero, Thanja Lamberts

29 **Molecular complexity in Solar-System analogs**
Eleonora Bianchi

30 **A Challenging Quest to Unveil the Beyond-the-Second-Period Chemistry in Space**
M. Michielan, D. Ascenzi, N. Balucani, G. Di Genova, and C. Ceccarelli

31 **Astrochemical Modeling of Protostellar Core Envelopes**
Prasanta Gorai, Jonathan C. Tan, and Yichen Zhang

32 **Comparing the Reactivity of HCN and $HCONH_2$ on Amorphous and Crystalline Mg_2SiO_4 Surfaces: Insights into Interstellar Dust Grain Chemistry**
Rosangela Santalucia , Erika Varesi, Guillermo Escolano Casado, Gloria Berlier, Giuseppe Spoto, Lorenzo Mino, Piero Ugliengo

33 **Chemical Evolution During the Formation of a FHSC: the B1b-N Case**
David Navarro-Almaida, Patrick Hennebelle, Benoît Commerçon, Maryvonne Gerin, Ugo Lebreuilly, and Asunción Fuente

34 **Chemical Environment Of Emerging Hot Cores: The Early Warm-Up Phase Chemistry**
Laure Bouscasse and Timea Csengeri

35 **Solid Interstellar Radical Chemistry (SIRC):**
A New Methodology to Study Radical Reactivity in Interstellar Ice Analogues
F. Duvernay, A. Gutiérrez-Quintanilla, Y. Layssac, T. Butscher, S. Henkel, Y.A. Tsegaw, D. Grote, W. Sander and T. Chiavassa

36 **Computational Approach for the High-Throughput Screening of Molecular Interactions for Prebiotic Astrocatalysis**
Eric Mates-Torres, Albert Rimola

37 **Constraining the Diffuse Envelope Surrounding L1544**
J. Ferrer Asensio, S. Spezzano, P. Caselli, S. Jensen, O. Sipilä, E. Redaelli, F. Alves

38 **Grain growth in star formation**
Pierre Marchand

39 **Ion-neutral reactions for formation and destruction of interstellar Complex Organic Molecules**
Daniela Ascenzi, Christian Alcaraz, Claire Romanzin, Roland Thissen, Vincent Richardson, David Sundelin, Wolf Geppert, Miroslav Polášek, Emília Valença, Ferreira de Aragão, Noelia Faginas-Lago, Marzio Rosi and Fernando Pirani

40 **Gas-Phase Formation Of Interstellar Methyl Cyanide: Review And New Theoretical Calculations**
L.Giani, C.Ceccarelli, L.Mancini, E.Bianchi, M. Rosi, F.Pirani and N.Balucani

41 **Formation and elongation of polyglycine via unimolecular reaction in the gas phase**
P. Bertier, H. Lissillour, L. Parrado Ospina, D. Comte, L. Lavy, P. Calabria, R. Fillol, F. Calvo, I. Daniel, B. Farizon, M. Farizon, T. D. Märk

42 **OMC-2 FIR4: a protostellar cluster full of surprises.**
L. Chahine, A. Lòpez-Sepulcre, R. Neri, S. Mercimek, L. Podio, C. Codella, C. Ceccarelli, P. Caselli and M. De Simone

43 **Molecular fractionation from clouds to planetary systems**
Eva Wirström

44 **First ALMA Maps of Cosmic-Rays Ionization Rate in High-mass Star-forming Regions**
Giovanni Sabatini , Stefano Bovino & Elena Redaelli

45 **A high HDO/H_2O ratio in the Class I protostar L1551 IRS5**
A. Andreu , A. Coutens, F. Cruz-Sáenz de Miera, N. Houry, J. K. Jørgensen, A. Kóspál and D. Harsono

46 **Formaldehyde In The Dynamic Protobinary System [BHB2007] 11: Deuteration and Streamer Kinematics**
Lucy Evans , Charlotte Vastel, Francesco Fontani, Jaime Pineda, Izaskun Jimènez-Serra, Mathilde Bouvier, Cecilia Ceccarelli and the FAUST team

47 **A study of the ^{13}C and ^{15}N fractionation in low-mass starless cores**
Sigurd S. Jensen, Silvia Spezzano, Paola Caselli, Elena Redaelli, Olli Sipilä, Judit Ferrer Asensio and Katharina Giers

48 **Formaldehyde Deuteration In The Young Disk of IRS 63: The Astrochemical Link To The Origin Of The Solar System**
Linda Podio , Dominique Segura-Cox, and the FAUST Team

49 **Chemical evolution from molecular clouds to star-forming regions, and beyond**
Yasuhiro Oba

50 **Combined hydrodynamic and gas-grain chemical modeling of star forming cores**
M. Bonfand and R. Garrod

51 **Heterogeneous Astrocatalysis. Mechanistic Studies For The Catalytic Formation Of iCOMs Based On Fischer-Tropsch Processes.**
Gerard Pareras & Albert Rimola

52 **Hydrogenation Of CO, H_2CO, And CH_3CHO Alongside NO In The Interstellar Medium**
J. Vitorino, E. Congiu, and F. Dulieu

53 **Origin of COMs Towards Hot Cores Selected from ALMA-IMF**
T. Csengeri , M. Bonfand, L. Bouscasse, T. Kushwahaa and ALMA-IMF collaboration

54 **Unravelling The Path to Molecular Complexity With Quantum Chemistry**
Isabelle Fourré, Chloé Simha, Anthony Fontana, Riccardo Spezia

55 **Unveiling chemical structures of star-forming regions with machine learning techniques**
Katharina Giers , Silvia Spezzano, Yuxin Lin, and Paola Caselli

56 **A Spatially Resolved Map of Cosmic Ray Ionization Rate and Electron Fraction**
Jaime E Pineda, O. Sipilä, D. M. Segura-Cox, R. Neri, M. Kuffmeier, M. T. Valdivia-Mena, M. J. Maureira, P. Caselli, S. Spezzano, S. S. R. Offner, N. Cunningham, A. Schmiedeke, and M. Chen

57 **The chemical composition of solar-type protostars with the ALMA large spectral surveys PILS and COMPASS**
Audrey Coutens, the PILS team and the COMPASS team

58 **Dimerization of HCN on Interstellar Silicates Grain Cores: A Quantum Mechanical Study**
Niccolò Bancone, Stefano Pantaleone, Piero Ugliengo, Marta Corno, Albert Rimola

59 **Astrochemically Relevant H-Atom-Abstraction and H-Atom-Addition Reactions Connecting Fulminic Acid (HCNO) and Formaldoxime (H_2CNOH)**
Barbara Keresztes, Sándor Góbi, István Pál Csonka, Gopi Ragupathy, Gábor Bazsó, and György Tarczay

60 **Protostellar shocked regions as factories of organic molecules: the case of L1157**
Ana López-Sepulcre, Claudio Codella, Linda Podio, Cecilia Ceccarelli, Nadia Balucani

61 **Super-Oxygenation of Naphthalene: The break-Down Reaction**
Dario Campisi

62 **The Effect Of Metallicity On The Abundances Of Molecules In Protoplanetary Disks**
Rodrigo Guadarrama, Eduard I. Vorobyov , Christian Rab , Manuel Güdel

63 **Where Planetary Systems Are Born Matters: The Chemistry Of Clustered Versus Isolated Environments And Cradle Of The Sun**
M. Bouvier, C. Ceccarelli, A. López-Sepulcre, N. Sakai, S. Yamamoto, Y.-L. Yang

64 **Collision Induced Dissociation of Water Pyrene Molecular Clusters**
A. Nair, S. Zamith, L. Toucouere, H. Leboucher, A. Simon, A. Marciniak, J.M. L’Hermite, C. Joblin

Posters

80 **Rearrangement Pathways to form Cyano-indene, an Interstellar PAH, and its Photoelectron Spectroscopic Characterization**
Mayank Saraswat, Adrian Portela-Gonzalez, Enrique Mendez-Vega, Ginny Karir, Patrick Hemberger, and Prof. Wolfram Sander

81 **Rivers in The Sky: Streamers Toward Two Embedded Sources in Perseus**
M. T. Valdivia-Mena , J. E. Pineda, D. M. Segura-Cox, and P. Caselli

82 **S(^{1}D) insertion reactions on the surface of ice mantles. An overlooked mechanism to form S-containing organic species?**
Gabriella Di Genova, Nadia Balucani, Andrea Giustini, Cecilia Ceccarelli, Marzio Rosi

83 **Spectroscopy of Small Phosphorus-Containing Molecules of Astrophysical Interest**
Elavenil Ganesan, Arun-Libertsen Lawzer, Thomas Custer, Jean-Claude Guillemin, and Robert Kołos

84 **The Chemical Composition Of A Protostellar Envelope With Luminosity Outbursts**
Pierre Marchand , Audrey Coutens, and Jules Scigliuto

85 **The Impact Of Luminosity Bursts On The Chemistry Of Protostars**
Antoine Espagnet , Audrey Coutens, and Pierre Marchand

86 **The S^+ + SiH_2 Reaction: Toward the Synthesis of Interstellar SiS**
L. Mancini , M. Rosi, D. Skouteris, F. Pirani, G. Di Genova, N. Balucani, C. Ceccarelli

LIST OF PARTICIPANTS

A
Aneesa Ahmad (a.ahmad@leeds.ac.uk)
Audrey Andreu (audrey.andreu@irap.omp.eu)
Christopher Arumainayagam (carumain@wellesley.edu)
Daniela Ascenzi (daniela.ascenzi@unitn.it)
Céline Assadourian (celine.assadourian@univ-amu.fr)

B
Nadia Balucani (nadia.balucani@unipg.it)
Niccolò Bancone (niccolo.bancone@uab.cat)
Vittorio Bariosco (vittorio.bariosco@unito.it)
Paul Bertier (p.bertier@ip2i.in2p3.fr)
Eleonora Bianchi (eleonora.bianchi@origins-cluster.de)
Mélisse Bonfand (pgu4gb@virginia.edu)
Laure Bouscasse (bouscasse@iram.fr)
Mathilde Bouvier (bouvier@strw.leidenuniv.nl)
Giulia Bovolenta (gbovolenta@udec.cl)

C
Dario Campisi (campisi@theochem.uni-stuttgart.de)
Stephanie Cazaux (S.M.Cazaux@tudelft.nl)
Cecilia Ceccarelli (cecilia.ceccarelli@univ-grenoble-alpes.fr)
Carla-Louise Chadourne (carla-louise.chadourne@univ-tlse3.fr)
Layal Chahine (layal.chahine@univ-grenoble-alpes.fr)
Steven Charnley (steven.b.charnley@nasa.gov)
Claudio Codella (codella@arcetri.astro.it)
Marta Corno (marta.corno@unito.it)
Audrey Coutens (audrey.coutens@irap.omp.eu)
Timea Csengeri (timea.csengeri@u-bordeaux.fr)

D
Marta De Simone (marta.desimone@eso.org)
Carlos del Burgo Olivares (cdelburgo@cab.inta-csic.es)
Gabriella Di Genova (gabriella.digenova@studenti.unipg.it)
Silvio Di Rosa (silvio.dirosa@inaf.it)
Francois Dulieu (francois.dulieu@cyu.fr)
Fabrice Duvernay (fabrice.duvernay@univ-amu.fr)

E
Joan Enrique Romero (j.enrique.romero@lic.leidenuniv.nl)
Guillermo Escolano Casado (guillermo.escolanocasado@unito.it)
Antoine Espagnet (antoine.espagnet@irap.omp.eu)
Lucy Evans (phyle@leeds.ac.uk)

F
M. Noelia Faginas Lago (noelia.faginaslago@unipg.it)
Judit Ferrer Asensio (ferrer@mpe.mpg.de)
Isabelle Fourré (isabelle.fourre@sorbonne-universite.fr)

G
Elavenil Ganesan (eganesan@ichf.edu.pl)
Lisa Giani (lisa.giani@univ-grenoble-alpes.fr)
Katharina Giers (kgiers@mpe.mpg.de)
Marie Gogibu (marie.gogibu@univ-grenoble-alpes.fr)
Prasanta Gorai (prasanta.astro@gmail.com)
Rodrigo Guadarrama (rodrigo.guadarrama@univie.ac.at)

H
Basile Husquinet (basile.husquinet@cyu.fr)

I
Alexei Ivlev (ivlev@mpe.mpg.de)

J
Sigurd Jensen (sigurdsj@mpe.mpg.de)
Christine Joblin (christine.joblin@irap.omp.eu)

K
Harjasnoor Kakkar (harjasnoor.kakkar@uab.cat)
Shreya Kakkenpara Suresh (shreyaks@mpe.mpg.de)
Barbara Keresztes (barbi1226@gmail.com)
Franciele Kruczkiewicz (franciele.kruczkiewicz@lam.fr)

L
Ngoc Tram LE (lengoctramlyk31@gmail.com)
Manuela Lippi (manuela.lippi@inaf.it)
Ana Lopez Sepulcre (lopez@iram.fr)

M
Arya M Nair (arya.nair@irsamc.ups-tlse.fr)
Luca Mancini (luca.mancini2@studenti.unipg.it)
Pierre Marchand (pierre.marchand.astr@gmail.com)
Berta Martínez Bachs (berta.martinez@uab.cat)
Eric Mates-Torres (eric.mates@uab.cat)
Andrés Megías (anmegias@ucm.es)
Matteo Michielan (matteo.michielan@unitn.it)

N
David Navarro (david.navarroalmaida@cea.fr)
Thanh Nguyen (nguyenthanh@lowtem.hokudai.ac.jp)
Michel Nuevo (michel.nuevo@nasa.gov)

O
Yasuhiro Oba (oba@lowtem.hokudai.ac.jp)

P
Stefano Pantaleone (stefano.pantaleone@unito.it)
Gerard Pareras (gerard.pareras@uab.cat)
Jessica Perrero (jessica.perrero@uab.cat)
Jaime Pineda (jaime.e.pineda@gmail.com)
linda podio (linda.podio@inaf.it)

R
Isabelle Ristorcelli (isabelle.ristorcelli@irap.omp.eu)
Marzio Rosi (marzio.rosi@unipg.it)

S
Giovanni Sabatini (giovanni.sabatini4@unibo.it)
Rosangela Santalucia (rosangela.santalucia@unito.it)
Mayank Saraswat (Mayank.Saraswat@ruhr-uni-bochum.de)
Jules Scigliuto (jules.scigliuto@irap.omp.eu)
Caroline Stadler (caroline.stadler@univ-amu.fr)

T
Patrice Theule (patrice.theule@lam.fr)
Alexander Tielens (tielens@strw.leidenuniv.nl)

U
Piero Ugliengo (piero.ugliengo@unito.it)

V
Maria Teresa Valdivia Mena (mvaldivi@mpe.mpg.de)
Charlotte Vastel (cvastel@irap.omp.eu)
Julie Vitorino (julie.vitorino@cyu.fr)

W
Valentine Wakelam (valentine.wakelam@u-bordeaux.fr)
Eva Wirström (eva.wirstrom@chalmers.se)
Qin Tong Wu (qw101@wellesley.edu)