BOOK OF ABSTRACTS

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Rationale and motivations

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 the actors of this intrinsically interdisciplinary endeavor: astronomers, chemists, and modelers. The recent huge progresses in the three areas make the time ripe for these communities to join and ride this scientific wave.

The conference aims to review:

- The new results from the powerful observing facilities, such as the IRAM-NOEMA, ALMA and VLA interferometers, and the chemical composition during the youngest phases of Solar-like planetary systems, from pre-stellar cores to protoplanetary disks, with particular emphasis on the interstellar complex organic molecules.
- The recent progresses due to the enhancement of high-performance computing facilities combined with efficient quantum chemistry algorithms, which allow for the *in-silico* simulation of many chemical processes occurring both in gas-phase and at grain surfaces.
- The latest laboratory experiments which have provided new insights on the possible processes occurring in the interstellar conditions.
- The new generation astrochemical models as well as the innovative tools to interpret the astronomical observations that have seen the light in the last few years.
- The most recent results on the chemical composition of the small bodies of the Solar System.

The conference is organised in the context of the EU 2020 ITN project **AstroChemical Origins (ACO)**

This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No **811312**.

DOC (Dawn of Organic Chemistry)

This project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (grant agreement No **741002**)

CONFERENCE PROGRAM

MONDAY 13-09-2021

10:00	**ARRIVAL & REGISTRATION**	
13:15	**Welcome**	
13:30	LOC	Opening talk

INTERSTELLAR ICES

Time	Speaker	Title
14:00	***M. McCoustra***	Experimental and Computational Laboratory Astrochemistry - A Personal View
14:30	A. Germain	Application of the Tight Binding GFN-xTB2 Method to Model Large Interstellar Amorphous Icy Grains
14:45	L. Tinacci	A New Approach to Compute Accurate Binding Energy Distribution of Complex Organic Molecules at Ice Interstellar Grain Models: the case of NH_3
15:00	S. Vogt-Geisse	A New Platform for Generating, Storing and Accessing High Quality Quantum Chemical Data of Molecular Binding Energies on Interstellar Icy Grain Surfaces
15:15	S. Ferrero	The Energy Dissipation Process of Hydrogenation Reactions of Atomic Nitrogen on Water Ice Surfaces
15:30	**COFFEE BREAK**	
16:30	G. Perotti	Ice and gas: linking infrared and millimeter observations towards solar-type protostars
16:45	F. Kruczkiewicz	Ammonia Snow Lines and Ammonium Salts Desorption
17:00	M. A. Corazzi	Thermal Desorption of Astrophysical Relevant Ice Mixtures of Acetaldehyde and Acetonitrile from Olivine Dust
17:15	L. Chu	Observations of Interstellar Ices in Pre-Solar Environments

TUESDAY 14-09-2021

INTERSTELLAR ICES

Time	Speaker	Title
09:00	***A. Boogert***	Ices in Solar-type Star Forming Regions
09:30	F. Duvernay	iCOM Formation from Radical Chemistry: a Mechanistic Study from Cryogenic Matrix Coupled with IR and EPR Spectroscopies
09:45	J. Enrique-Romero	Radical-Radical chemistry on amorphous icy surfaces
10:00	G. Molpeceres	Neural-Network Assisted Study of H_2 adsorption on solid CO
10:15	S. Pantaleone	H_2 and HCO· formation on interstellar grains and the fate of reaction energy
10:30	**COFFEE BREAK**	
11:30	A. Dehghanfar-Witzel	Interstellar icy mantle formation in molecular clouds
11:45	M. De Simone	Tracking Ice Mantle History in Solar-type Protostars

MOLECULAR COMPLEXITY

12:00	***J. Cernicharo***	QUIJOTE: Q-band Ultrasensitive Inspection Journey to the Obscure TMC-1 Environment
12:30	**LUNCH**	
14:30	C. Zhou	Molecular complexity in the cold ISM: Influence of the environment
14:45	I. Jimenez-Serra	Formation, Abundance Distribution and Evolution of Complex Organic Molecules in Starless/Pre-stellar Cores
15:00	G. Sabatini	The first survey of ortho-H_2D^+ in high-mass star-forming regions
15:15	X. He	Destruction routes of interstellar molecules: collisions of He^+ with CH_3OH
15:30	**COFFEE BREAK**	
16:30	S. Demes	Collisional excitation of H_3O^+ by H_2: towards better understanding of interstellar water chemistry
16:45	V. Richardson	Gas-Phase Reactivity of $[CNH_3]^+$ Ions of Relevance to the Ionosphere of Titan
17:00	L. Tychoniec	Which molecule traces what? Chemical diagnostics of protostellar sources revealed with ALMA
17:15	L. Mancini	Probing the Chemistry of P-Bearing Molecules in Interstellar and other Extraterrestrial Environments
17:30	E. Piacentino	Modeling of the chemical evolution of PO_x and HPO_x (x=2,3) on icy grains

WEDNESDAY 15-09-2021

MOLECULAR FRACTIONATION

Time	Speaker	Title
09:00	***N. Balucani***	Gas-phase chemistry in the interstellar medium: there is still much to learn
09:30	***P. Caselli***	Molecular fractionation in star- and planet-forming regions
10:00	L. Evans	Nitrogen Fractionation Towards the Protocluster OMC-2 FIR4
10:15	L. Colzi	Carbon Isotopic Fractionation in Molecular Clouds
10:30	**COFFEE BREAK**	
11:30	A. Lopez-Sepulcre	Protostellar shocks as factories of formamide (NH_2CHO), a key prebiotic precursor
11:45	P. Nazari	Complex Organic Molecules from Low- To High-Mass Protostars
12:00	A. Schutzer	Molecules in Protostellar Jets: Lessons from CepE-mm
12:15	P. R. Rivera-Ortiz	A numerical study of CO kinematics in the CepE-mm Molecular Outflow
12:30	**LUNCH**	

THURSDAY 16-09-2021

COMETARY ICES

Time	Speaker	Title
09:00	***S. Tachibana***	What do pristine Solar System materials tell us about the origin and early evolution of the Solar System?
09:30	***D. Bockelee-Morvan***	The composition of cometary ices
10:00	E. Bianchi	The astrochemical link between Sun-like protostars and Solar System comets
10:15	L. Podio	The Chemistry of Planet-Forming Disks with ALMA-DOT: towards a comparison with comets to unveil the origin of the Solar System
10:30	**COFFEE BREAK**	

MOLECULAR COMPLEXITY

11:30	***R. Martin-Domenech***	Experimental simulations of Complex Organic Molecule formation in the ISM (with a little help from theory)
12:00	R. Santalucia	Reactivity of Gaseous HCN at Amorphous and Crystalline Mg_2SiO_4 Surfaces as Laboratory Models of Interstellar Dust Grains
12:15	O. El Samrout	Role of specific silica surface sites in the promotion of peptides formation
12:30	**LUNCH**	
14:30	B. Maté	Urea in Astrophysical Environments: IR Spectra and Destruction Cross Sections for Energetic Processing
14:45	M. Saitta	Step by Step Strecker Amino Acid Synthesis from Ab Initio Prebiotic Chemistry
15:00	M. Bouvier	The chemical nature of Orion protostars: Are ORANGES different from PEACHES?
15:15	A. Belloche	Questioning the spatial origin of complex organic molecules in young protostars with the CALYPSO survey
15:30	**COFFEE BREAK**	
16:30	L. Chahine	Organic Chemistry in The Proto-Solar Analogue OMC-2 FIR 4: Environment Matters
16:45	R. Le Gal	Impact of C/O on the chemistry of PDRs and protoplanetary disks
17:00	M. van Gelder	Modeling accretion shocks at the disk-envelope interface: sulfur chemistry
17:15	M. Ali-Dib	A correlation between the chemistry and eccentricity of hot TNOs
20:00	**SOCIAL DINNER**	

FRIDAY 17-09-2021

MOLECULAR COMPLEXITY

Time	Speaker	Title
09:30	F. Vazart	Gas-phase Formation of Acetaldehyde: Review and New Theoretical Computations
09:45	D. Gonzalez	Insights On the Gas-Phase OH+CH_3NH_2 Reaction: Experimental Rate Coefficients at Interstellar Temperatures (21.7-177.5 K)
10:00	E. Valenca Ferreira de Aragao	Kinetics Studies of The Cyanoacetylene and Atomic Oxygen Reaction
10:15	J. Zamponi	A Hot Gravitationally Unstable Disk as The Origin of The Class 0 Hot Corino IRAS 16293-2422 B
10:30	**COFFEE BREAK**	
11:30	N. Tanha	The effects of episodic accretion on the chemistry of the protostellar discs and envelopes
11:45	S. Mercimek	Chemical Inventory of Class I Protostars: A Bridge Between Protostellar Cores and Protoplanetary Disks
12:00	A. Waggoner	X-ray Flare Driven Chemical Evolution in Planet Forming Regions
12:15	C. Law	Chemical Substructures at 10 au Scales in Protoplanetary Disks: Results from the Molecules with ALMA at Planet-forming Scales (MAPS) Large Program
12:30	V. M. Rivilla	Prebiotic precursors of nucleic acids, proteins, and sugars in Solar-like protostars
12:45	LOC	Closing remarks

ORAL CONTRIBUTIONS

A correlation between the chemistry and eccentricity of hot TNOs

Mohamad Ali-Dib[1] , Michael Marsset, Wing-Cheung Wong and Rola Dbouk

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We investigate the origins of the photometrically Very Red and Less Red Trans-Neptunian Objects. We first re-analyze the dataset of Marsset et al. (2019) and find that, in addition to the known color-inclination correlation in hot TNOs, a similar trend exists for color-eccentricity. We show that VRTNOs are sharply constrained to eccentricities < 0.42 and inclinations < 21◦, leading to a paucity of VR scattered disk and distant MMR objects. We then interpret these findings using N-body simulations accounting for Neptune's outward migration into a massless particles disk, and find that these observations are best reproduced with a LR-to-VR color transition line between ∼ 38 and 42 AU in the primordial disk, separating the objects' formation locations. For an initial surface density profile ($\Sigma \propto 1/r2$), a color transition around 38 AU is needed to explain the high abundance of VR plutinos but creates too many VR scattered disk objects, while a transition line around 42 AU seems to better reproduces the scattered disk colors but creates virtually no VR plutinos.

Gas-phase chemistry in the interstellar medium: there is still much to learn

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In addition to the formation of hydrides on the surface of the icy mantles of interstellar grains,[1] it has been recently proposed that the entire set of interstellar complex organic molecules is actually formed by radical-radical recombination processes assisted by interstellar ice.[2] However, many gas-phase reactions have been previously overlooked and their inclusion in astrochemical models can significantly improve the model predictivity. In particular, it has been recently verified that the presence of a pre-reactive complex can strongly promote the reactivity at very low temperatures for several reactions characterized by a significant energy barrier.[3] In addition, the deuteration of interstellar complex organic molecules can be well explained by gas-phase processes,[4] while ice chemistry fails to do so.[5]
In this review talk, I will present some of the most recent achievements on gas-phase chemistry that might provide a new twist in our comprehension of the chemical evolution of interstellar objects.

Acknowledgements: This research was supported by the Italian Space Agency (ASI, DC-VUM-2017-034, Grant No 2019-3 U.O Life in Space) and the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie project grant agreement No 811312 for the project "Astro-Chemical Origins" (ACO).

1. S. Cazaux, A.G.G.M. Tielens, C. Ceccarelli et al., *Astrophys. J.*, **2003**, 593, L51.
2. RT Garrod, SL Widicus Weaver, E Herbst *Astrophys. J.* **2008,** 682, 283.
3. A. Potapov, A. Canosa, E. Jimenez, B. Rowe, *Angew. Chem. Int. Ed*. **2017**, 56, 8618.
4. D. Skouteris, F. Vazart, C. Ceccarelli *et al*, *MNRAS* **2017**, 468, L1
5. J.K. Jorgensen, H.S.P. Muller, H. Calcutt *et al*. *Astronom. Astrophys.* **2018**, 620, A170

Questioning the Spatial Origin of Complex Organic Molecules in Young Protostars with the CALYPSO Survey

Arnaud Belloche[1] , and the CALYPSO collaboration

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Complex organic molecules (COMs) have been detected in a few Class 0 protostars but their spatial origin is not well understood. In addition to probing the chemical processes that lead to molecular complexity during the protostellar evolution, these molecules may also trace physical processes such as heating, accretion, and ejection. We have used the CALYPSO survey performed with the Plateau de Bure Interferometer to search for COMs at high angular resolution in a sample of 26 solar-type protostars. I will report on the results of this investigation[1] which has, in particular, revealed a chemical differentiation in multiple systems that is markedly different from the case of the prototypical binary system IRAS16293-2422.

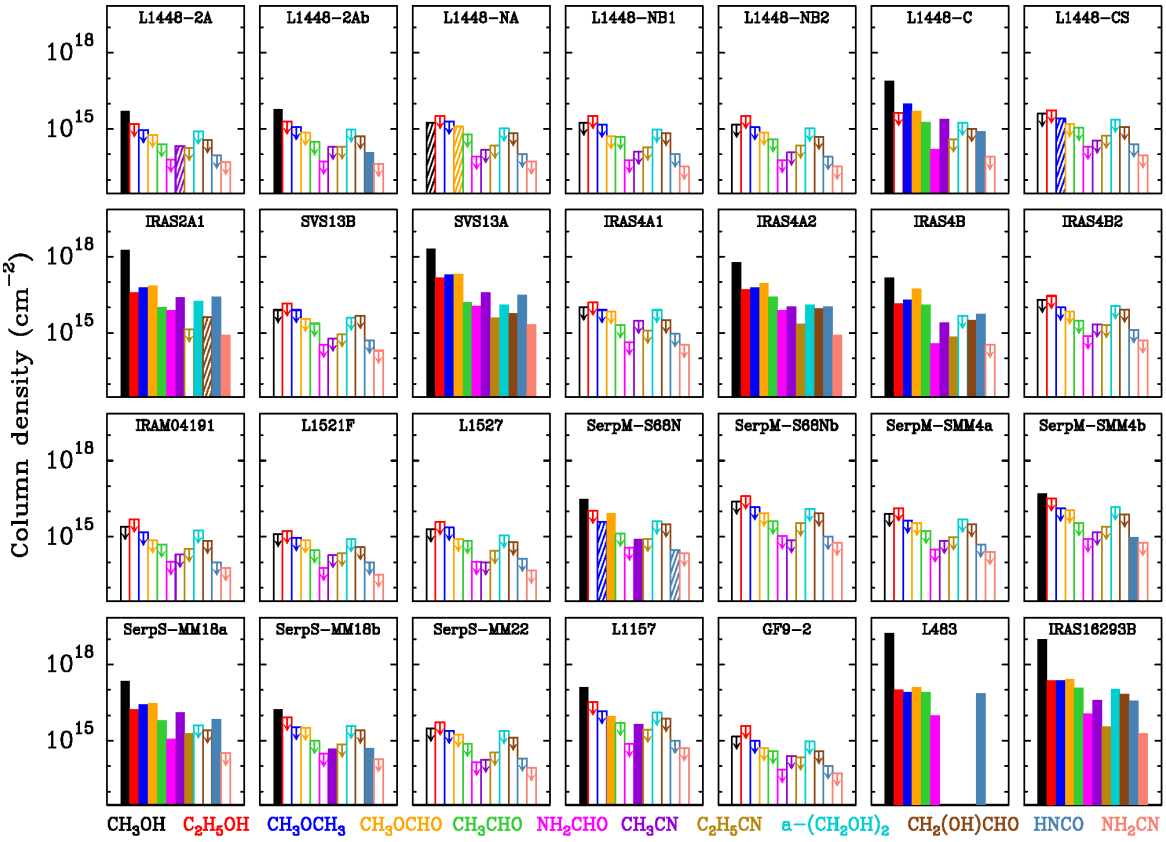

Figure 1: *Column densities of (complex) organic molecules toward CALYPSO sources, compared to Class 0 protostars L483 and IRAS16293B.*

1. A. Belloche, A. J. Maury, S. Maret, et al., *Astronomy & Astrophysics*, **2020**, 635, A198

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

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Observations of complex organic molecules in cometary ices give us information about the most pristine known material from which our Solar System formed[1]. Comparing the observed astrochemical content in young protostars with that in comets is a powerful way to start answering questions like: 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 there is a complete chemical reset?
An example is provided by the recent comparison of young disks composition with the chemical census obtained towards the comet 67P thanks to the ROSETTA mission[2,3,4].

I will present a chemical systematic study of a few Class I sources obtained in the framework of three IRAM and ALMA Large Programs: ASAI, SOLIS and FAUST. The different datasets offer the opportunity to sample the different spatial scales, up to the planet formation region (~ 50 au). The first comparative studies show striking correlations for the abundance ratios of some complex organic molecules like $HCOOCH_3$, CH_3OCH_3 and C_2H_5OH, suggesting clues of inheritance from the protostellar phase[4,5]. These new observations represent a first test of the inheritance scenario from the protostellar phase.

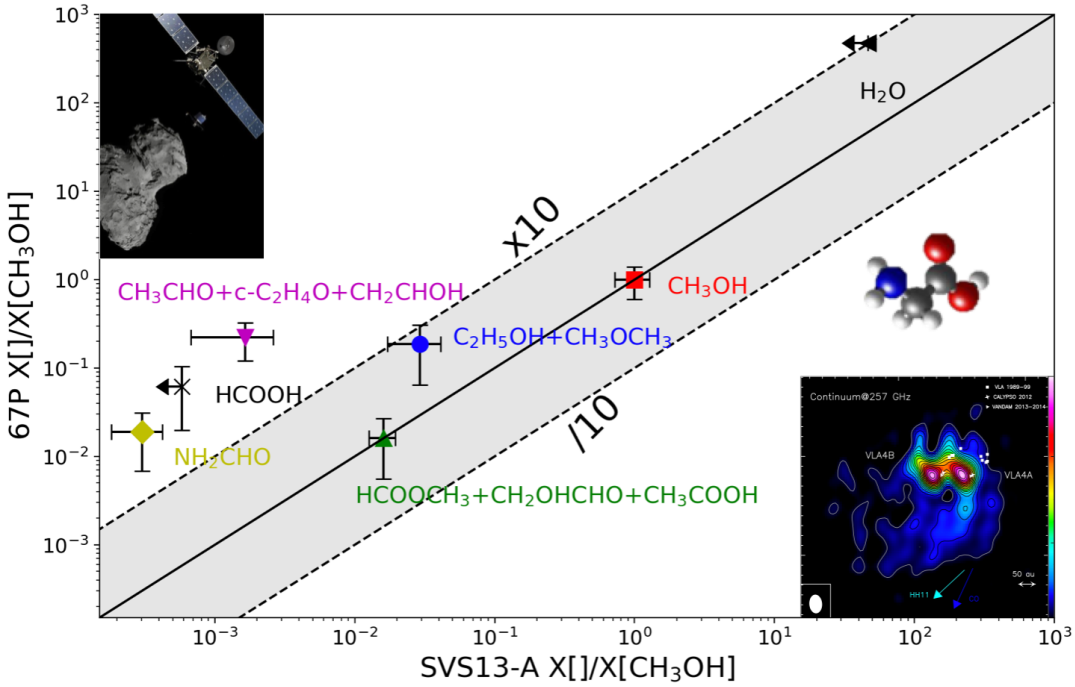

Figure 1: *Preliminary comparison between the chemical complexity of a Class I protostar and the comet 67P. The present results will be updated in the light of the new SOLIS and FAUST observations*

1. K. Altwegg, H. Balsiger, S. A. Fuselier, *Annual Review of Astronomy and Astrophysics*, **2019,** 57, 113-155

2. M. Rubin, C. Engrand, C. Snodgrass, P. Weissman, K. Altwegg, H. Busemann, A. Morbidelli, M. Mumma, *Space Science Reviews,* **2020**, 216, 102

3. E. Bianchi, C. Codella, C. Ceccarelli, F. Fontani, L. Testi, R. Bachiller, B. Lefloch, L. Podio, V. Taquet, *Monthly Notices of the Royal Astronomical Society,* **2019**, 483, 1850

4. M. N. Drozdovskaya, E. F. van Dishoeck, M. Rubin, J. K. Jørgensen, K. Altwegg, *Monthly Notices of the Royal Astronomical Society,* **2019**, 490, 50-79

5. E. Bianchi, C. Chandler, C. Ceccarelli, C. Codella, N. Sakai, et al., *Monthly Notices of the Royal Astronomical Society,* **2020**, 498, L87-L92

The Composition of Cometary Ices

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The composition of cometary ices provides clues to the chemistry and conditions prevailing in the early solar system. Since the detection of HCN at millimeter wavelengths in comet C/1973 E1 (Kohoutek), almost 30 molecules have been identified in cometary atmospheres including complex organic molecules, from remote sensing observations from ground or space platforms. More recently, the *in-situ* investigation of comet 67P/Churyumov-Gerasimenko by the Rosetta mass spectrometers revealed a wealth and variety of new volatile compounds, from unexpected simple species, like O_2, to complex prebiotic molecules as glycine. Measurements will be reviewed and discussed with respect to the origin of cometary ices.

Figure 1: *Comet C/2020 F3 (NEOWISE) on 12 July 2020 – Credit Lukas Vesely*

Ices in Solar-type Star Forming Regions

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A stunning variety of volatiles has been detected in comet 67P/Churyumov-Gerasimenko by the Rosetta mission[1]. The origin of ices in this and other comets is debated. The question of the dense cloud heritage can to a certain degree be constrained by infrared spectroscopy of ice bands towards dense clouds and low mass protostars. While the number of interstellar ice species detected this way is fundamentally limited by the overlap of vibrational modes, I will show that great progress can be expected with the capabilities offered by the James Webb Space Telescope[2], which will be launched soon. I will discuss how the ice bands are used to trace ice processing in the environments of low mass protostars, and the importance of laboratory experiments in this regard. This will be illustrated with recent NASA IRTF observations of ices toward massive protostars. The comparison of ice properties in low and high mass protostars is insightful because of their different formation histories and physical conditions.

1. K. Altwegg, H. Balsiger, S.Fuselier, *ARAA*. **2019**, 57, 113
2. A. Boogert, P. Gerakines, D. Whittet, *ARAA*. **2015**, 53, 541

The chemical nature of Orion protostars: Are ORANGES different from PEACHES?

M. Bouvier[1] , C. Ceccarelli[1,2], A. López-Sepulcre[1,3], N. Sakai[4], S. Yamamoto[5,6], Y.-L. Yang[7,4]

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[2]*CNRS, IPAG, F-38000 Grenoble - FRANCE*

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The protostellar stage is known to be chemically rich and diverse. Indeed, molecules that were trapped onto the ice mantles of grains during the prestellar core phase are released into the gas phase, resulting in the chemical enrichment and diversity of the protostar environment[1,2] Key pieces of evidence of this chemical diversity are hot corinos and Warm Carbon Chain Chemistry (WCCC) objects, two chemically distinct types of solar-mass protostars. On the one hand, hot corinos are compact (<100 au), dense ($n>10^7$ cm^{-3}) and hot (>100 K) regions[3,4], enriched in interstellar Complex Organic Molecules (iCOMs; e.g. CH_3OH, CH_3OCH_3)[5,6]. On the other hand, WCCC protostars have an inner region deficient in iCOMs but a larger zone (~1000 au) enriched in hydrocarbons (e.g. CCH, c-C_3H_2). This protostellar chemical diversity could reflect a difference in the chemical composition of the grains ice mantle set during the pre-stellar core phase. Whether the environment affects this diversity and how, is still an open question.

In order to understand what causes the chemical diversity of solar-type protostars, we need to perform systematic studies of the chemical composition of solar-mass protostars at small scales located in different environments. In this context, two recent studies were performed. The first one is the Perseus ALMA Chemistry Survey (PEACHES)[7] which targeted a relatively loose protocluster, containing only low-mass objects. The second one is the ORion ALMA New GEneration Survey (ORANGES)[8], which targeted the Orion Molecular Cloud 2/3 filament, the nearest low- to high- mass star forming region, highly UV illuminated by nearby HII regions. While the PEACHES study showed that hot corinos were likely dominant in Perseus, I will present the new results obtained from the ORANGES, which show that, indeed, ORANGES are different from PEACHES.

1. Cazaux et al., *ApJ*. **2003**, 593, 51
2. Jørgensen et al., *A&A*. **2016,** 595, 117
3. C. Ceccarelli, *ASPC*. **2004**, 323, 195
4. C. Ceccarelli et al., *PPV*. **2007**, 47
5. E. Herbst & E. F. van Dishoeck, *ARA&A*. **2009**, 47, 427
6.C. Ceccarelli et al., *ApJ*. **2017**, 850, 176
7. Y.-L. Yang et al. *ApJ*, **2021**, 910, 20
8. M. Bouvier et al. *in prep*

Molecular fractionation in star- and planet-forming regions

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Our Solar System has kept record of the earliest phases of its evolution, at the time when all current ingredients were dispersed in a dense molecular cloud, the pre-stellar cloud core. This is testified by the similarities between the chemical composition of primitive material, such as comets and carbonaceous chondrites, and that of young protostars, where the pre-stellar ices have just evaporated. Of particular interest are the D and ^{15}N fractionation processes in H- and N-bearing molecules present at the various phases of star- and planet-formation, as they provide information on the chemical journey from clouds to planets, thus our astrochemical origins. In this review talk, I will summarize our current understanding of D- and ^{15}N-fractionation in molecular material from clouds to protoplanetary disks and highlight puzzles.

QUIJOTE: Q-band Ultrasensitive Inspection Journey to the Obscure TMC-1 Environment

J. Cernicharo[1], M. Agúndez,[1], C. Cabezas[1], B. Tercero[2], J.R. Pardo[1], Marcelino[1], P. deVicente[2]

[1]*Institute of Fundamental Physics (CSIC). Group of Molecular Astrophysics, C/Serrano 121, Madrid, Spain*

[2]*Centro Astronómico de Yebes, Observatorio Astronómico Nacional, Yebes, Guadalajara, Spain*
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We present a line survey of the cold dark core TMC-1 carried out with the YEBES 40m radio telescope (see Figure 1) in the Q-band. A new set of receivers have been installed in the telescope within the frame of the ERC synergy Nanocosmos project that allows to cover the whole 31-50 GHz band in dual polarization. The spectral resolution is 38.15 kHz. The sensitivity achieved so far varies between 0.2 and 1.0 mK, and allows to search for new molecules in a line by line (no stacking) detection procedure. These new data have permitted to detect the protonated species HC_5NH^+ [1], HC_3O^+ [2], HC_3S^+ [3], and CH_3CO^+ [4]. Each one of these species were detected first in TMC-1 by looking for unknown lines with harmonic frequency relations. All of them have been confirmed in the laboratory except HC_5NH^+, for which our identification is based in high-level of theory ab initio calculations. Neutral molecules with low permanent dipole moment such as CH_2CHCCH [5], $CH_2CCHCCH$ [6], and C_3H_3 [7] have been also detected and have a very large abundance. Finally we show our detection of the cycles cyclopentadiene, ethynyl cyclopropenylidene, and indene [8], the first PAH detected in space. We discuss the chemistry of these species and in particular the possible reactions leading to the formation of these cycles.

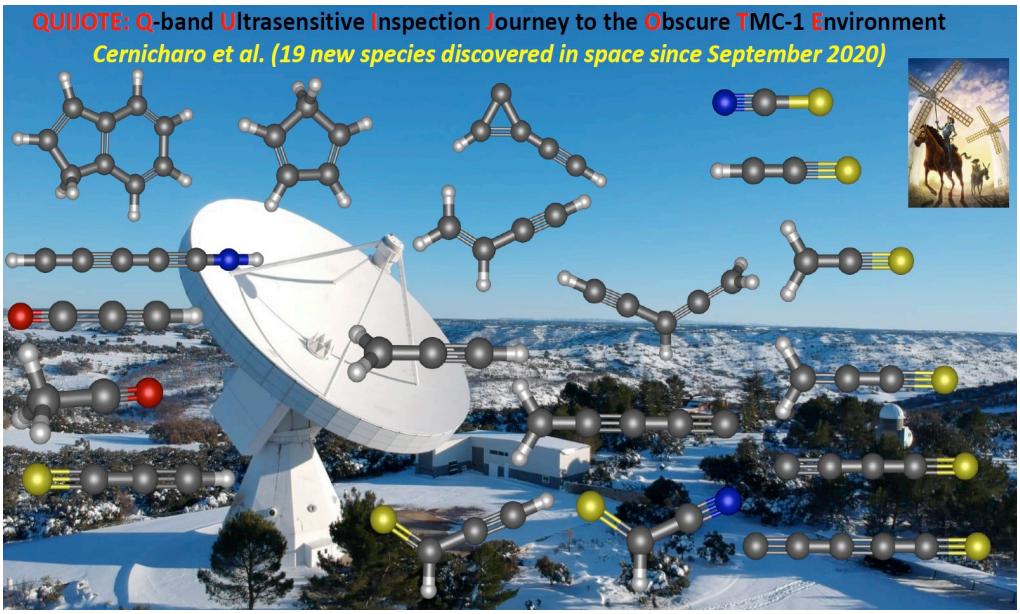

Figure 1: *The Yebes 40m telescope with the 19 molecules detected since September 2020*

[1] Marcelino et al. 2020, A.&A., 643, L6
[2] Cernicharo et al. 2020, A.&A., 642, L17
[3] Cernicharo et al. 2021, A.&A., 643, L3
[4] Cernicharo et al. 2021, A.&A., 646, L7
[5] Cernicharo et al. 2021, A.&A., 647, L2
[6] Cernicharo et al., 2021, A.&A., 647, L3
[7] Agúndez et al., 2021, A&A, 647, L10
[8] Cernicharo et al., 2021, A&A, 649, L15

Organic Chemistry in the Proto-Solar Analogue OMC-2 FIR 4: Environment Matters.

L. Chahine[1,2], A. Lòpez-Sepulcre[1,3], R. Neri[1], S. Mercimek[4,5], C. Codella[4,3], L. Podio[4], C. Ceccarelli[3], M. Bouvier[3], E. Bianchi[3,4], C. Favre[3], N. Sakai[6] and S. Yamamoto[7]

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Hot corinos are compact regions around solar-mass protostellar objects that are very rich in interstellar Complex Organic Molecules (iCOMs)[1,2]. They are believed to represent the very early phases of our Solar System's birth, which was very likely also characterized by rich organic chemistry. While most of the studied hot corinos are either isolated or born in a loose proto-cluster, our Sun was born in a densely packed star cluster, near massive stars whose ultraviolet radiation must have contributed to shaping the evolution of the surrounding environment[3]. In addition, internal irradiation from energetic particles (>10 MeV), whose imprint is seen today in the products of short-lived radionuclides in meteoritic material, is also known to have occurred during Solar System formation[4]. How all these conditions affected the chemistry of the proto-Sun and its immediate surroundings is still an open question.

To answer this question, and in the framework of the H2020 MSCA ITN Project AstroChemical Origins (www.aco-itn.org), we will present recent results on HOPS-108, the hot corino located in the proto-solar analogue OMC-2 FIR 4[5]. The study was carried out with ALMA at 1.3mm with a spatial resolution of ~100 AU. We detected 11 iCOMs such as CH_3OH, $HCOOCH_3$ and CH_3OCH_3. Our results can be summarised as follows: (1) a significant enhancement of $HCOOCH_3$ with respect to other hot corinos, (2) a $[CH_3OCH_3]/[HCOOCH_3]$ abundance ratio of ~0.2 deviating from the usual trend seen in other sources ($[CH_3OCH_3]/[HCOOCH_3]$ ~1), (3) a $[CH_2DOH]/[CH_3OH]$ ratio of ~2.5% which is lower than what is seen in Perseus and Ophiuchus hot corinos (~7%-9%) and similar to that seen in HH212, which, as HOPS-108, is a protostellar source located in Orion[6].

The third result was the basis for a recently submitted follow-up ALMA proposal aiming to study molecular deuteration in this source and investigate if it deviates from what is usually seen in other hot corinos, as that may be a consequence of having protostars formed in a high-mass cloud environment.

References:

1. Ceccarelli, C. 2004, in Astronomical Society of the Pacific Conference Series, Vol. 323
2. Caselli, P. & Ceccarelli, C. 2012, A&A Rev., 20, 56
3. Adams, F. C. 2010, ARA&A, 48, 47
4. Gounelle, M., Chaussidon, M., & Rollion-Bard, C. 2013, ApJ, 763, L33
5. Chahine, L., Lòpez-Sepulcre, A., Neri, R., et al. In preparation
6. Bianchi, E., Codella, C., Ceccarelli, C., et al. 2017, A&A, 606, L7

Observations of Interstellar Ices in Pre-Solar Environments

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Dense molecular cores provide ideal environments for the growth of ices and complex organic molecules (COMs) on the cold surfaces of dust grains. Some of these early molecules are essential in building the foundation for planetary systems and may even survive the harsh planetary formation process[1]. From the recent flyby of the undisturbed Kuiper Belt Object, Arrokoth by the New Horizons mission, we know that methanol ice (CH_3OH) may have formed early in the pre-solar environment[2,3]. CH_3OH is a possible precursor to forming other COMs[4] and until now, it has been difficult to observationally constrain the conditions (e.g. local cloud densities, time scales) or the efficiency governing COM growth. Here we present L and M band spectroscopy from five dense molecular cores, which were probed by observing nine background stars and five Class II YSOs. Using the SpeX instrument on the NASA Infrared Telescope Facility (IRTF), we obtained absorption bands of the following ices from the cloud cores: H_2O (3.0 μm), CH_3OH (C-H stretching mode, 3.53 μm), and CO (4.67 μm). For the first time, the detections of both CO and CH_3OH through lines of sight toward background stars observationally constrain the conversion of CO into CH_3OH ice. This allows us to test whether COMs can form in the pre-stellar cold environments without energetic particle interactions (e.g. cosmic rays). In order to understand the conditions under which these ices form, we have developed high spatial resolution (~13-29") extinction maps of each molecular core using infrared JHK band observations made from WFCAM on the United Kingdom Infrared Telescope (UKIRT) and IRAC channels 1 and 2 from the *Spitzer Space Telescope*. Using a new computational tool, AVIATOR[5], we implement the inverse Abel transform allowing us to develop three-dimensional maps of the cores to calculate the *volume densities* of total hydrogen along the lines of sight where ices are detected. We will present the volume density thresholds determined for different ices to form and the fraction of each core that is dense enough for COMs to develop on dust grains. This work is in preparation for the large-scale ice maps that will be obtained with the 3-5 μm slitless spectroscopy mode of NIRCAM on JWST (part of a GTO program) and will be important for the interpretation of spectroscopic features in the 5-26 μm region of these cores from approved JWST Cycle 1 programs as well.

[*] *NASA Postdoctoral Program Fellow*

1. Visser, R., van Dishoeck, E. F., Doty, S. D., & Dullemond, C. P. **2009**, *A&A*, 495, 881
2. Stern, S. A., Weaver, H. A., Spencer, J. R., et al. **2019,** *Science*, 364, aaw9771
3. Grundy, W. M., Bird, M. K., Britt, D. T., et al. **2020**, *Science*, 367, aay3705
4. Fedoseev, G., Chuang, K. J., Ioppolo, S., et al. **2017**, *ApJ*, 842, 52
5. Hasenberger, B., & Alves, J. **2020**, *A&A*, 633, A132

Carbon Isotopic Fractionation in Molecular Clouds

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Understanding isotopic fractionation over a large scale, from terrestrial oceans, meteorites, planetary, and cometary atmospheres up to Galactic and extragalactic is crucial[1]. One element for which fractionation is important is carbon. In fact, in molecular clouds a $^{12}C/^{13}C$ ratio found from galactocentric gradients, which only considers the formation of the two elements via stellar nucleosynthesis, is commonly assumed. However, this value is improperly used since it was shown by theoretical models that the $^{12}C/^{13}C$ ratio also depends by the physical conditions of molecular clouds, such as densities, temperatures and cosmic-ray ionization rate. In this talk I will review the C-fractionation chemical models of the literature.

In particular, chemical models predict that low-temperature isotopic exchange reactions may lead to ^{13}CO and $H^{13}CO^+$ enrichment towards starless and pre-stellar cores[2], which are thought to be pre-Solar nebula analogs. This results in a dilution of ^{13}C in the other gas-phase molecular species, and $^{12}C/^{13}C$ ratios two times higher than those observed across the Galaxy (~68 in the local interstellar medium).

Moreover, I will present the gas-grain chemical network we have implemented with new isotopic exchange reactions and the effects of their introduction in the context of dense and cold molecular gas[3]. We suggest a possible ^{13}C exchange through the $^{13}C + C_3 \rightarrow {}^{12}C + {}^{13}CC_2$ reaction, which leads to $^{12}C/^{13}C$ ratios that tend to 68, or lower values, for molecules that are formed starting from atomic carbon. Moreover, we investigated the $^{12}C/^{13}C$ ratios of HNC, HCN, and CN using a grid of models, with temperatures and densities ranging from 10 to 50 K and 2×10^3 to 2×10^7 cm^{-3}, respectively. One of the main results is that we are able to marginally reproduce some of the observed values towards low-mass pre-stellar cores[4,5]. Finally, we studied the $^{12}C/^{13}C$ ratios of nitriles by varying the cosmic-ray ionization rate. This is the first work of carbon fractionation that includes the effect of a gas+grain chemistry and new isotopic-exchange reactions.

1. P. Caselli & C. Ceccarelli, *The Astronomy and Astrophysics Review*. **2012**, 20, 56

2. E. Roueff, J. C. Loison, K. M. Hickson, *Astronomy and Astrophysics.* **2015**, 576, A99

3. L. Colzi, O. Sipilä, E. Roueff, P. Caselli, F. Fontani, *Astronomy and Astrophysics.* **2020**, 640, A51

4. F. Daniel, M. Gérin, E. Roueff, J. Cernicharo, N. Marcelino, F. Lique, D. C. Lis, D. Teyssier, N. Biver, D. Bockelée-Morvan, *Astronomy and Astrophysics.* **2013**, 560, A3

5. V. S. Magalhães, P. Hily-Blant, A. Faure, M. Hernandez-Vera, F. Lique, *Astronomy and Astrophysics.* **2018**, 615, A52

Thermal Desorption of Astrophysical Relevant Ice Mixtures of Acetaldehyde and Acetonitrile from Olivine Dust

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Millimeter and centimeter observations are discovering an increasing number of interstellar complex organic molecules (iCOMs) in a large variety of star-forming sites from the earliest stages of star formation[1] to protoplanetary disks[2].

In this context, it is pivotal to understand the influence of the solid phase interactions between iCOMs and grain surface in the thermal desorption process and the subsequent presence of molecular species in the gas phase. In laboratory, it is possible to simulate the thermal desorption process deriving important parameters such as the desorption temperatures and energies. Up to now, temperature-programmed desorption (TPD) experiments have been carried out mainly from graphite and amorphous water ice surfaces[3,4,5,6], although mineral matrices can selectively adsorb, protect, and allow the iCOMs concentration on their surface.

We report our new recently published laboratory results[7] on TPD experiments of astrophysical relevant ice mixtures of water, acetonitrile, and acetaldehyde from olivine grains used as interstellar dust analog on which the icy mixtures were condensed at 17 K. We found that in the presence of grains, only a fraction of acetaldehyde and acetonitrile desorbs at about 100 K and 120 K respectively, while 40% of the molecules are retained by fluffy grains of the order of 100 μm up to temperatures of 200 K. In contrast with the typical assumption that all molecules are desorbed in regions with temperatures higher than 100 K, this result implies that about 40% of the molecules can survive on the grains enabling the delivery of volatiles towards regions with temperatures as high as 200 K and shifting inwards the position of the snowlines in protoplanetary disks. These studies offer a necessary support to interpret observational data and may help our understanding of iCOMs formation providing an estimate of the fraction of molecules released at various temperatures.

1. G. A. Blake, E. C. Sutton, C.R. Masson, T.G. Phillips, *ApJ.* **1987**, 315
2. J. Lee, S. Lee, G. Baek et al., *Nature Astronomy.* **2019**, 3
3. M. P. Collings, M. A. Anderson, R. Chen et al., *MNRAS.* **2004**, 354
4. T. Hama, N. Watanabe, A. Kouchi & M. Yokoyama, *ApJL.* **2011**, 738
5. J. Shi, G. A. Grieves & T. M. Orlando, *ApJ.* **2015**, 804
6. H. Chaabouni, S. Diana, T. Nguyen & F. Dulieu, *A&A.* **2018**, 612
7. M. A. Corazzi, J. R. Brucato, G. Poggiali, L. Podio, D. Fedele & C. Codella, accepted on *ApJ.* **2021**

Tracking Ice Mantle History in Solar-type Protostars

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Solar-type planetary systems are formed from cold clumps where dust grains are covered with mantles of iced molecules. The species relative abundances in the mantles depend on the clump physical conditions and the chemical budget at the onset of gravitational collapse[1,2,3]. Since the species in the mantles govern the chemical complexity of the future forming objects, their composition is of paramount importance for the eventually formed planetary system.

The major components of the dust grain mantles have been estimated to be, via infrared (IR) observations, H_2O, CO, CO_2, CH_4, NH_3 (ammonia), CH_3OH (methanol) plus other molecules with smaller abundances[4]. However, these observations can be done only for sources that have sufficiently bright IR continuum emissions. In particular, retrieving the composition of the icy mantles of very young Solar-type protostars has been impossible so far.

Once the gravitational collapse starts, the temperature near the central object rises, heats the surrounding dust, and the species trapped in the mantles sublimate becoming observable with radio-mm facilities[5]. Then, NH_3 and CH_3OH become the critical tracers of the ice mantle composition as CO is often optically thick and confused with the surrounding cloud, CO_2 and CH_4 do not have permanent dipole moments, and H_2O is difficult to observe from the ground due to the atmosphere. Additionally, being NH_3 and CH_3OH well known grain surface products[6,7], the evolution of their abundances only depends on the mantle formation history and, therefore, their observed values can be compared with predictions, as the ones in Figure 1.

We observed NH_3 and CH_3OH with the VLA interferometer toward a sample of protostars in the Perseus/NGC 1333 region, in order to perform a multiline analysis to accurately derive their molecular abundances and the gas properties. We will show how the derived NH_3/CH_3OH abundance ratio allows us to trace the ice mantle history of the observed sources, constraining the clump temperature and the ice mantle formation time scale.

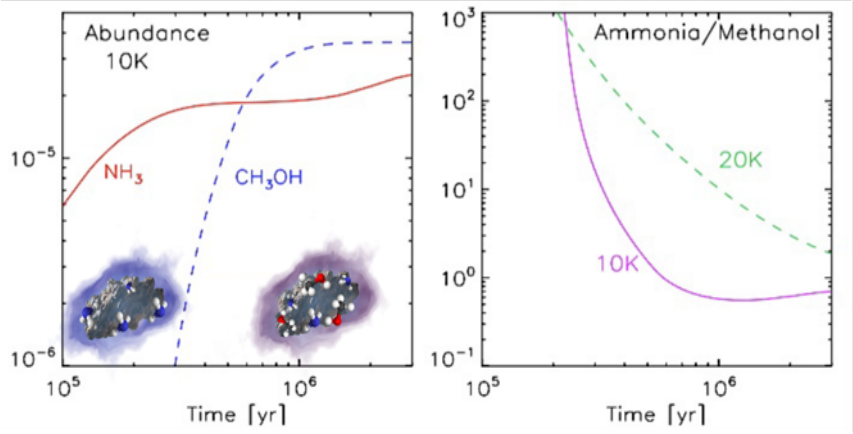

Figure 1 *Theoretical predictions of***:** *(left) NH_3 and CH_3OH abundance in the grain mantles vs time for a clump with temperature of 10 K; (right) NH_3/CH_3OH abundance vs time for clump temperatures of 10 and 20 K.*

1. V. Taquet, A. López-Sepulcre, C. Ceccarelli et al., *ApJ*, **2012**, 748, L3
2. H.M. Cuppen, C. Wlash, T. Lamberts, et al. *SSRev*, **2017**, 212,1
3. M. N. Drozdovskaya, C. Walsh, E. Van Dishoeck, et al. *MNRAS, **2016**, 462, 977*
4. A.C.A. Boogert et al. 2015, *ARAA*, **2015**, 53, 541
5. P. Caselli & C. Ceccarelli, A&ARv, **2012**, 20, 56
6. N. Watanabe & A. Kouchi, *ApJ*, **2002**, 571, L173
7. A. Rimola, V. Taquet, P. Ugliengo, et al. *A&A*, **2014**, 572, 70

Collisional excitation of H_3O^+ by H_2: towards better understanding of interstellar water chemistry

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Hydronium cations (H_3O^+) have been detected in both dense and diffuse molecular clouds of the interstellar medium (ISM)[1], where they play a crucial role in oxygen and water chemistry. While the spectroscopy of H_3O^+ was intensively studied earlier[2], there are only limited works devoted to its collisional excitation by interstellar colliders[3,4]. Nevertheless new, accurate rate coefficients for the collisions involving H_3O^+ are obviously needed.

We studied the rotational excitation of hydronium cations by collisions with H_2 for the first time from a close-coupling method. Our recent, highly correlated 5D potential energy surface[5] is used to describe the collisional system. State-to-state inelastic cross sections were computed and the corresponding thermal rate coefficients were obtained for kinetic temperatures up to 300 K. Both the *ortho*- and *para*- nuclear spin isomers of the H_3O^+ were considered. The calculated rates are to be used to estimate the abundance of interstellar hydronium, which can lead to a better understanding of interstellar water chemistry.

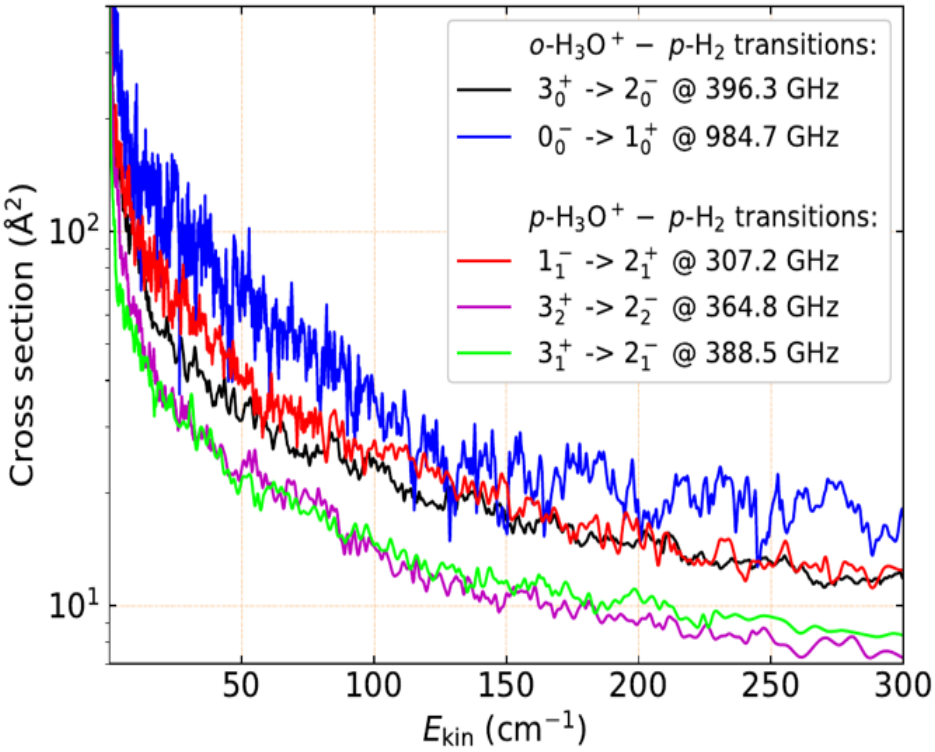

Figure 1: *Rotational de-excitation cross sections for collision of ortho- and para-H_3O^+ with para-H_2 as a function of kinetic energy.*

1. F. F. S. Van Der Tak, S. Aalto, R. Meijerink, *Astron. Astrophys*. **2008**, 477, L5.
2. V.V. Melnikov, S. N. Yurchenko, J. Tennyson, P. Jensen, *Phys. Chem. Chem. Phys.* **2016**, 18, 26268.
3. H. El Hanini, F. Najar, M. Naouai, N.-E. Jaidane, *Phys. Chem. Chem. Phys.* **2019**, 21, 11705.
4. A. R. Offer and M. C. van Hemert, *Chem. Phys.* **1992**, 163, 83.
5. S. Demes, F. Lique, A. Faure, C. Rist, J. Chem. Phys. 2020, 153, 094301.

iCOM Formation from Radical Chemistry: a Mechanistic Study from Cryogenic Matrix Coupled with IR and EPR Spectroscopies.

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Interstellar complex organic molecules (iCOMs) have been identified in different interstellar environments including star forming regions as well as cold dense molecular clouds[1]. Laboratory studies show that iCOMs can be formed either in gas-phase or in the solid state, on icy grains, from "non-energetic" (atom-addition/abstraction) or energetic (UV-photon, particle bombardments) processes[2-4]. In this contribution, using a new experimental approach mixing matrix isolation technique, mass spectrometry, and infrared and EPR spectroscopies, we want to investigate the COM formation at 35 K from a complex mixture of ground state radicals trying to draw a general reaction scheme. We photolyze (121 nm) CH_3OH diluted in Ar at low temperature (below 15 K) to generate HCO, HOCO, CH_2OH, CH_3O, OH and CH_3 radicals and "free" H-atoms within the matrix. Radicals have been identified using infrared and EPR spectroscopies. With the disappearance of the Ar matrix (at 35 K), these unstable species are then free to react, forming new species in a solid film. Some recombination products have been detected using infrared spectroscopy and mass spectrometry in the solid film after Ar removal, namely methyl formate (CH_3OCHO), glycolaldehyde ($HOCH_2CHO$), ethylene glycol ($HOCH_2CH_2OH$), glyoxal (CHOCHO), ethanol (CH_3CH_2OH), formic acid (HCOOH), dimethyl ether (CH_3OCH_3), methoxymethanol (CH_3OCH_2OH) and CH_4O_2 isomers (methanediol and/or methyl hydroperoxide). The detected molecules are fully consistent with the radicals detected and strongly support the solid-state scenario of iCOM formation in interstellar ices based on radical-radical recombination. We then discuss astrophysical implications of the radical pathways on the observed gas-phase iCOMs.

1. B.A. McGuire, *ApJS*. **2018**, 239, 17

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

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

4. N. Abou Mrad, F. Duvernay, T. Chiavassa, G. Danger, *MNRAS*. **2016**, 458, 1234

Role of specific silica surface sites in the promotion of peptides formation

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This work is dedicated to the memory of Prof. Gianmario Martra who designed this work but left us suddenly.

Silica based minerals are amongst the most studied materials with regard to the formation of the first biomolecules due to their ubiquitous presence in many environments, such as interstellar dust grains and the Earth's crust. Indeed, the interaction of silicate surfaces with amino acids has been proposed, and experimentally confirmed, as a mechanism for peptide formation, indicating the relevance of silica minerals in both abiotic and prebiotic chemistry[1]. The possibility of polymerization reactions on the surface of space dust grains would be confirmed by the recent discovery of a protein analogue (hemolithin, involving chains of glycine and hydroxy-glycine residues) inside a meteorite[2]. The interaction of biomolecules with amorphous silica (SiO_2) represents an intriguing case study for materials science, due to the complexity of the silica surface, exposing both hydrophobic and hydrophilic portions[3].

In this contribution, the mechanism of the catalytic formation of polyglycine (Gly) on the surface of amorphous silica is elucidated by IR and mass spectrometry, focusing on the reactivity of strained silica rings (3 or 4-membered), pre-reacted with formic acid. The reaction proceeds through two steps: (i) silica ring opening by reaction with formic acid to form a Si-O-C-(=O)- surface mixed anhydride (SMA) with a subsequent hydrolysis of surface species by the adsorption of water vapor and (ii) reaction of the SMA with Gly adsorbed through chemical vapor deposition (CVD) to form the poly-Gly chains. The results suggest a high selectivity of the structure of the silica surface that catalyzes the polymerization of Gly: only one sub-family of Si-OH surface groups (nearly-free silanols located around 5 Å apart) are active toward peptides formation. Parallel experiments carried out on amorphous silica untreated with formic acid result in less abundant and shorter oligomers. Furthermore, the results show the mobility of the poly-Gly on the surface when contacted with water vapor to form organized self-assembled structures. The work also indicates that the polypeptides formed by condensation of Gly on the silica are linked to the surface by covalent bonds resulting in their strong resistance to desorption when washing with liquid water.

1. A. Rimola, D. Costa, M. Sodupe, J. F. Lambert, & P. Ugliengo, *Chemical Reviews*. **2013**, 6, 4216-4313

2. M. McGeoch, S. Dikler, &, J. E. McGeoch. *ArXiv preprint arXiv*. **2020**, 2002.11688.

3. R. J. Gillams, & T. Z. Jia, *Life*, **2018**, 8, 10.

Radical-Radical Chemistry on Amorphous Water Surfaces

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Understanding how interstellar complex organic molecules (iCOMs) are formed and destroyed is of high importance to predict the ultimate organic complexity reached in the interstellar medium (ISM)[1,2]. Two paradigms are invoked in the literature: the first assumes that hydrogenated species in the interstellar ice mantles of dust particles lead to the formation of iCOMs once they are released to the gas phase while the other states that iCOMs are formed on these ices due to the coupling of radical species formed out of the photodissociation of hydrogenated species inside the ice. The latter paradigm is nowadays the most popular among astrochemical models, even though some basic assumptions of the paradigm are still a topic of debate. Among them, the radical-radical reactivity assumption, which is extremely difficult to simulate and prove experimentally. We proposed an alternative/complementary method: theoretical quantum chemistry calculations, which can provide a precious atomistic perspective from which to study such processes[3,4,5].

In this contribution, we present our recent quantum chemical study reactivity of several radical pairs (e.g. CH_3 + CH_3, HCO + HCO, CH_2OH + CH_2OH, CH_3 + CH_2OH, HCO + CH_2OH among others) on the amorphous water surface (AWS). According to the observational evidence, the interstellar icy mantles are dominated by amorphous water[6]. We, therefore, simulated the ices with a model including 33 water model which possesses a cavity-like structure, where the effect of the larger number of intermolecular interactions on radicals can be investigated[4].

We computed the potential energy surfaces of several radical-radical reactions and their reaction efficiencies with the most accurate possible numerical methods presently available. For each radical pair, two reaction channels are found: radical couplings (leading to iCOMs) and direct H-abstractions (leading to simpler species as HX + Y → X + HY, where HX, Y are radicals). The occurrence of one process or the other could entirely depend on the relative orientation of the radicals upon encounter, namely on the water ice structure and interaction with the two radicals. Our results indicate that the fraction of iCOMs generated in the current astrochemical models is certainly overestimated since (i) it is assumed that reactions have efficiency of unity (ii) the competitive reactions often are not included.

1. E. Herbst. & E. F. van Dishoeck, *ARA&A*. **2009**, 47, pp. 427-480

2. C. Ceccarelli, P. Caselli, F. Fontani et al., *ApJ*. **2017**, 850, pp. 176

3. J. Enrique-Romero, A. Rimola, C. Ceccarelli et al., *MNRAS: Letters*. **2016**, 459(1), pp. 6-10

4. A. Rimola, D. Skouteris, N. Balucani et al., *ACS Earth Space Chem*. **2018**, 2(7), 720-734

5. J. Enrique-Romero, A. Rimola, C. Ceccarelli, et al., *ACS Earth Space Chem*. **2019**, 3(10), 2158-2170

6. Boogert, A. A., Gerakines, P. A., & Whittet, D. C., *ARA&A.* **2015**, 53, 541-581

Nitrogen Fractionation Towards The Protocluster OMC-2 FIR4

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The variety of the 14N/15N ratios found across the Solar System and beyond represents one of the biggest mysteries in astrochemistry. We investigated this variation in one of the closest and better analogues of the environment in which the Solar System was born - the protocluster OMC-2 FIR4 - using the first comparison at high angular resolution between HCN and N2H+ using interferometric data. Specifically, we observed the transitions H13CN (1-0) and HC15N (1-0) with the NOrthern Extended Millimeter Array (NOEMA) within the context of the IRAM Seeds Of Life In Space (SOLIS) Large Program. Our results show a small regional variation of the 14N/15N ratio for HCN from ~250-500. The ratios in the central regions of FIR4, where the candidate protostars are located, are largely consistent among them (~300). They also show little variation from the part of the protocluster known to harbour a high cosmic ray ionisation rate, to the portion with lower rate. These results suggest that local changes in the physical parameters occurring on small linear scales in the protocluster, including a high irradiation from cosmic rays, do not seem to affect the 14N/15N ratio in HCN. To better investigate this, we combined our results with analysis on archival data consisting of observations of N2H+ and its 15N-isotopologues using the Atacama Large Millimeter Array (ALMA). From this further analysis, we found a small variation in the 14N/15N ratio of N2H+ from ~200 to ~400. Therefore, we concluded tentatively that the nitrogen isotopic ratio does not vary on the small scales probed by our observations independently of the molecule used. This result suggests that the mechanisms previously claimed to regulate the 14N/15N ratio such as selective photodissociation do not seem to have any effect at the scales studied in this work; moreover, the high level of locally produced cosmic rays do not affect the N-fractionation.

Kinetics Studies of the Cyanoacetylene and Atomic Oxygen Reaction

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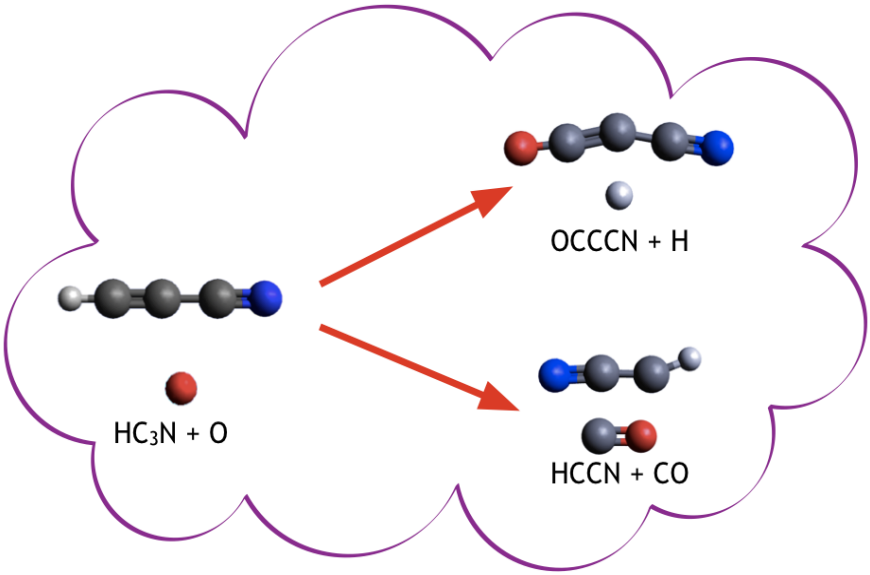
The 2018 census published by McGuire[1] reports that 204 molecular species have been detected in the interstellar medium up to this date. Understanding the processes involving the formation and destruction of those molecules is an important step to build astrochemical models.

In this work we present the results of a computational study on the reaction involving cyanoacetylene and atomic oxygen. This reaction has been previously investigated by Xie et al.[2] in the gas phase and on a water ice model. Based on the energetics, the authors have concluded that the reaction involving O (^{3}P) in the gas phase generates two products: OC_3N + H (major) and ^{3}HCCN + CO (minor). Meanwhile, the reaction involving O (^{1}D) generates mainly ^{1}HCCN + CO. Nevertheless, no value for the rate coefficient of product formation has been reported in that work or elsewhere.

In the present work we have reproduced the triplet and singlet potential energy surface of the reaction in the gas phase and two points of intersystem crossing. Electronic structure calculations have been performed employing the B3LYP[3] density functional for the geometry optimization and CCSD(T)[4] for the energetics. We will discuss the challenges and the eventual results of the kinetic studies on this reaction.



1. B. A. McGuire, *ApJS.* **2018**, 239, 17
2. H. Xie, Y.-H. Ding, C.-C. Sun, *Astrophys. J.* **2006**, 643, 573-581
3. A.D Becke, *J. Chem. Phys.* **1993**, 98(7), 5648–5652
4. R. J. Bartlett, *Annu. Rev. Phys. Chem.* **1981**, 32(1), 359–401

The Energy Dissipation Process of Hydrogenation Reactions of Atomic Nitrogen on Water Ice Surfaces

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In the colder (10-20K) regions of interstellar medium, the icy surfaces of interstellar grains serve as solid state supports for chemical reactions.[1] Among the plausible roles of these surfaces, that of third body is advocated, in which the formation energy of surface reactions can be dissipated among the grain causing the stabilization of the product.[2] This energy dissipation process is poorly understood at the atomic scale and it can have a tremendous impact on astrochemical surface processes like chemical desorption and diffusion.[3,4] In this work, we studied the formation of NH_3 via successive H-addition to atomic nitrogen on crystalline and amorphous ice surfaces. We first characterized the potential energy surfaces of the hydrogenation reactions and of possible competitive processes (i.e., H abstractions) using static quantum chemical calculations. Subsequently, the partitioning of the nascent energy released by the hydrogenation reactions between the newly formed species and the surface has been elucidated by means of *ab initio* molecular dynamics (AIMD) simulations. Results indicate that the H-additions on N are largely favorable reactions at 10 K, being barrierless and exhibiting large negative reaction energies, as opposed to the competitive H-abstractions, which are either endothermic or present high activation energies. AIMD simulations show that such favorable nascent energies are, in large part, quickly absorbed by the ice surfaces and their dissipation can be accelerated by mechanisms which involve an H exchange between the surface and the newly formed species.

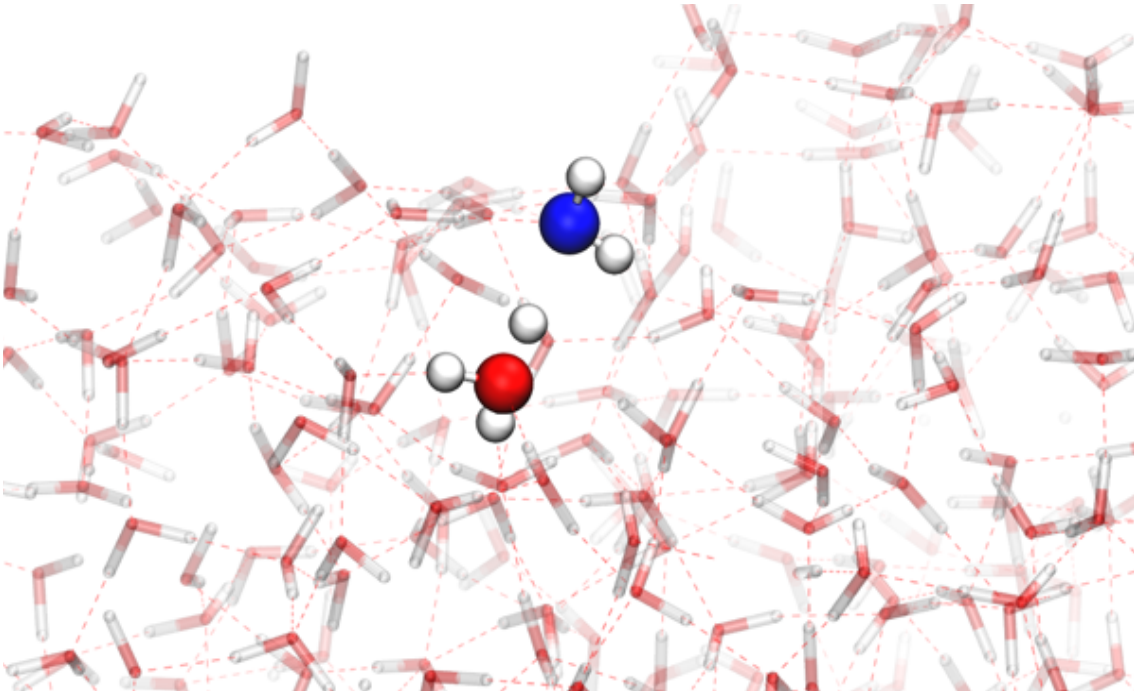

Figure 1: $H_3O(+)$ NH_2**(-)** *complex formation on an amorphous ice surface*

1. A. Potapov and M. McCoustra, *International Reviews in Physical Chemistry,* **2021**, arXiv preprint
2. G. Vidali, *Chem. Rev.* **2013**, 113, 12, 8762-8782
3. S. Pantaleone et al. *ApJ*, **2021,** arXiv preprint
4. S. Pantaleone et al. *ApJ*, **2020,** 897, 1, 56

Application of the Tight Binding GFN-xTB2 Method to Model Large Interstellar Amorphous Icy Grains

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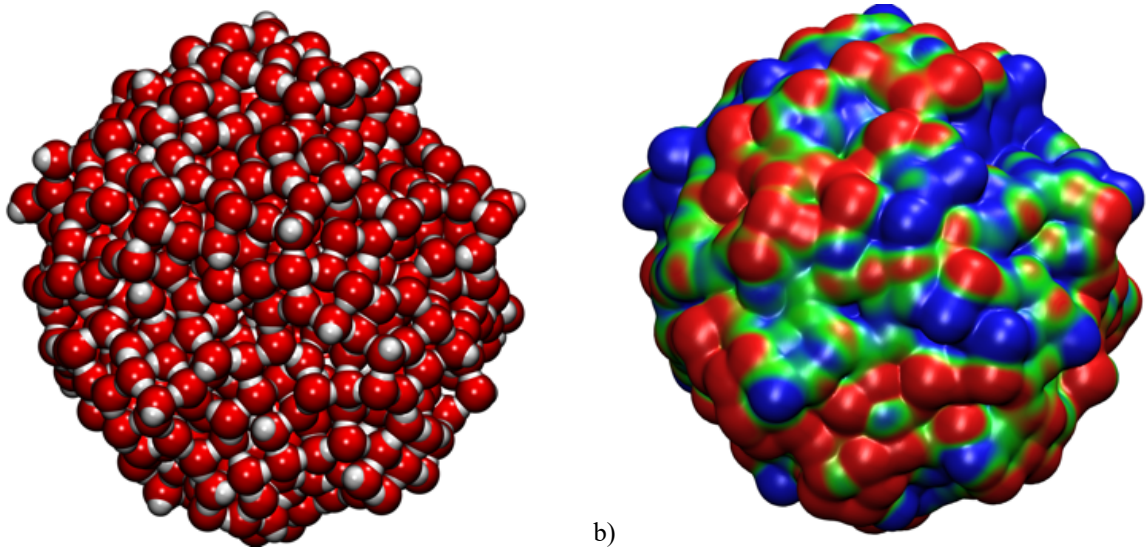
Interstellar grains are made of a silicate core covered by a mantle of several layers of amorphous ice. In the gas-phase of dense molecular clouds chemical species freeze onto the grain and can diffuse on its surface, react to give interstellar more complex molecules and ultimately desorb back to the gas-phase. Hence, the study of interstellar grains is an important part for understanding the chemical evolution in time of the Interstellar Medium (ISM). There is still no consensus in the Astrochemistry community on how to model these icy grains at atomistic level with the requisite of treating the hydrogen bond interaction and other important components accurately. Furthermore, the grain should be large enough to be representative of the variability present in the ISM, which renders impractical the adoption of plain DFT methods. Also, the adopted method should, not only be relatively fast, but also applicable to study the interaction of large interstellar molecules with the grain itself. Force fields are not the proper solution, due to the parametrization specific for each considered species, breaking the universality of the approach. To fill in the above requested, we resort to a newly developed semi-empirical quantum mechanical method based on the tight binding DFT approach called GFN-xTB2[1] and a universal force field method called GFN-FF[2], both developed by the Grimme's group at the Bonn University. We present the methodology to build a water cluster model up to 1000 H_2O molecules and to characterize its structural and electrostatic potential surface (EPS) as a free grain (Fig. 1). Then, NH_3 was chosen as relevant interstellar molecule to compute its binding energy (BE) at more than 150 different grain sites to characterize the BE distribution which revealed a bimodal distribution.



a) b)

Figure 1: *a) Structure and b) EPS of the xTB-GFN2 water cluster model (1000 H_2O)*

1. C. Bannwarth, S. Ehlert, S. Grimme, *J. Chem. Theory Comput.* **2019**, 15, 1652-1671

2. S. Spicher, S. Grimme, Angew. *Chem. Int. Ed.* **2020**, 59, 15665-15673

Insights on the Gas-Phase OH+CH_3NH_2 Reaction: Experimental Rate Coefficients at Interstellar Temperatures (21.7-177.5 K)

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The hostile conditions present in the interstellar medium (ISM), *i.e.* the space between two star systems, have not been an obstacle to detecting more than 200 different species of molecules[1]. In the coldest regions (~10 K) of the ISM, *i.e.* the dense molecular clouds, just a few complex organic molecules (COMs) have been observed. Some of them contain C-O or C-N bonds, which are considered potential precursors of prebiotic molecules, such as sugars or amino acids[2]. For example, methylamine (CH_3NH_2) was first detected in 1974 in Sgr B2 and Ori A[3]. Understanding the gas-phase chemistry of CH_3NH_2 at ultra-low temperatures is of great importance to elucidate the formation of other species, such as CH_3NH or CH_2NH_2 radicals, which can further contribute to the formation of larger COMs. One of the reactions to consider is the reaction of CH_3NH_2 with hydroxyl (OH) radicals, first detected in 1963[4] and ubiquitous in the ISM.

In this work, the experimental kinetics of the gas-phase reaction between CH_3NH_2 and OH have been studied between 21.7 K and 177.5 K for the first time, using the most powerful pulsed CRESU (French acronym for Reaction Kinetics in a Uniform Supersonic Flow[5]) worldwide. The CRESU technique is based on supersonic expansions through a specifically designed Laval nozzle. The OH radicals are generated in the cooled jet by pulsed laser photolysis (PLP) of H_2O_2 and the OH temporal profile is monitored by laser induced fluorescence (LIF). The study has been extended at temperatures between 263 K and 373 K with a conventional PLP-LIF system[6] to obtain a complete picture. An increase of the rate coefficient as the temperature decreases was observed in the investigated temperature range. The complete results will be presented and discussed at the conference.

1. D. E. Woon, http://www.astrochymist.org/astrochymist_ism.html

2. N. Balucani, *Int. J. Mol. Sci*. **2009**, 10, 2304-2335.

3. N. Kaifu, M. Morimoto, K. Nagane, K. Akabane, T. Iguchi, K. Takagi, *Astrophys. J.* **1974**, 191, 135-137

4. S. Weinreb, A. H. Barrett, M. L. Meeks, J. C. Henry, *Nature*. **1963**, 200, 829-831

5. E. Jiménez, B. Ballesteros, A. Canosa, T. M. Townsend, F. J. Maigler, V. Napal, B. R. Rowe, J. Albaladejo. *Rew. Sci. Ins*. **2015**, 86, 045108.

6. S. Blázquez, M. Antiñolo, O. J. Nielsen, J. Albaladejo, E. Jiménez. *Chem. Phys. Lett*. **2017**, 687, 297-302

Destruction routes of interstellar molecules: collisions of He^+ with CH_3OH

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Collisions between charged species (cations) and neutral molecules are often barrierless, hence they are expected to occur with high rates at the low temperatures characteristics of pre-stellar and proto-stellar regions. Ion-molecule reactions can play a role not only in the formation but also in the destruction of interstellar complex organic molecules (iCOMs)[1].

Helium is the second most abundant element in the Universe and it can be ionized by cosmic rays to generate helium cations. Due to the larger ionization energy of He with respect to organic molecules, collisions with He^+ are an important pathway for the destruction of iCOMs.[1] Methanol (CH_3OH) is one of the most abundant and ubiquitous among iCOMs and it has been widely observed in the gas phase in cold regions, where it is formed through continuous hydrogenation of CO (second most abundant gaseous molecule) by H/H_2 on the ice mantle or interstellar dust.[2] In the case of He^+ collisions, rate constants with several iCOMs are not available in the literature and quite often educated guesses are used in astrochemical models.[3] As previously shown for the case of dimethyl ether and methylformate[1], such estimates and extrapolations should be taken with a pinch of salt and experimental determinations coupled with theoretical modelling are fundamental to obtain consistent data to build-up reliable astrochemical models of iCOMs abundances.

In ion–molecule reactions, a possible channel is that triggered by charge transfer, a non-adiabatic process whose dynamics is governed by transitions occurring at the crossings between different intermolecular potential-energy surfaces (PESs) associated with states of the system differing for the exchange of one electron.[4,5]

Here we present recent experimental results on the collisions of He^+ with CH_3OH. A home-built guided ion beam mass spectrometer (GIB-MS) with O1-Q1-O2-Q2 configurations (where Q stands for Quadrupole and O stand for Octopole) is used to measure absolute integral cross sections and branching ratios as a function of the collision energy in the range from few meV to ~10 eV. The main product channels (in order of decreasing abundances) are:

$$\begin{aligned} He^+ + CH_3OH \quad &\rightarrow HCO^+ (m/z\ 29) + H_2 + H + He \\ &\rightarrow CH_3O^+/CH_2OH^+ (m/z\ 31) + H + He \\ &\rightarrow CH_3^+ (m/z\ 15) + OH + He \\ &\rightarrow CH_2^+ (m/z\ 14) + H_2O(OH+H) + He \end{aligned}$$

1. D. Ascenzi, A. Cernuto, N. Balucani, P.Tosi, C. Ceccarelli, L. M. Martini, F. Pirani, A&A. **2019**, 625.
2. E. Herbst, E. F. van Dishoeck, Annual Review of Astronomy and Astrophysics **2009**, 47 (1), 427-480.
3. O. Martinez, T. P. Snow, V.M. Bierbaum, Proceedings of the International Astronomical Union **2008**, 4, 139-140.
4. A. Cernuto, P. Tosi, L. M. Martini, F. Pirani, D. Ascenzi, Phys Chem Chem Phys **2017**, 19, 19554-19565.
5. A. Cernuto, F. Pirani, L. M. Martini, P. Tosi, D. Ascenzi, Chem Phys Chem **2018**, 19, 51-59.

Formation, Abundance Distribution and Evolution of Complex Organic Molecules in Starless/Pre-stellar Cores

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Observations carried out toward starless and pre-stellar cores have revealed that complex organic molecules (COMs) are prevalent in these objects (Vastel et al. 2014; Jimenez-Serra et al. 2019; Scibelli et al. 2020). However, it remains unclear what chemical processes are involved in COM formation and at what stage in dense core evolution complex organics form. In this contribution, we will present high-sensitivity observations carried out toward the L1517B and L1498 starless cores. These cores are believed to be at earlier evolutionary stages than the well-known L1544 pre-stellar core, also studied in COM emission by our group. Similarly to what we found in L1544, small O-bearing molecules and N-bearing species are enhanced by factors ~4-14 toward the outer shells of L1498 and L1517B. However, unlike L1544, large O-bearing COMs such as CH3CHO, CH3OCH3 or CH3OCHO are not detected within our sensitivity limits - comparable to the ones obtained for L1544. Surprisingly, N-bearing organics are more abundant toward the outer shells of L1498 and L1517B than in L1544. We have carried out a detailed modelling of the formation of O-bearing and N-bearing COMs in L1498 and L1517B following the model of Vasyunin et al. (2017), which considers both the chemical reactive desorption of COM precursors and their subsequent gas-phase chemistry yielding COMs. The distribution of the COM abundances predicted for L1498 and L1517B nicely matches our observations for both O-bearing and N-bearing COMs in these cores, and reveal that the differences observed between the complex organic content in L1498, L1517B and L1544 are due to the different physical structure of these cores, which in turn is a consequence of their evolution. From our results we conclude that while N-bearing COMs form early in dense core evolution, O-bearing COMs form at a later stage when enough CO has catastrophically depleted onto the surface of dust grains.

1. Vastel, C., Ceccarelli, C., Lefloch, B., & Bachiller, R. *ApJ,* **2014**, 795L, 2V

2. Jimenez-Serra, I., et al. *ApJ,* **2016**, 830L, 6J

3. Scibelli & Shirley, *ApJ,* **2020**, 891, 73S

Ammonia Snow Lines and Ammonium Salts Desorption

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Nitrogen depletion at different stages of star formation is a long-standing problem. It is likely that some of the nitrogen content is in the solid phase of cold regions, as in pre-stellar cores or protoplanetary disks mid-planes, and returns to the gas phase when this material is heated, for example in active comets. How and when this material will return to the gas phase or if it remains in a refractory content depends on the chemical nature of the nitrogen reservoir and its chemical environment. Ammonia desorption when present in an icy water matrix should occur at the same time as water desorption[1]. However, ammonia in its protonated form, NH_4^+, presents a more refractory character[2] and could remain on the surface of the dust grains until higher temperatures. The temperature dependence on the location of these different N reservoirs, in relation to water and methanol snow lines, is a step towards understanding planetary formation[3]. To support observations and in situ space missions, it is important to characterize the desorption process of these different nitrogen carriers, in addition to their temperature dependent IR spectra.

In this work, we experimentally investigated the desorption kinetics of two ammonium salts, ammonium formate and ammonium acetate. In our set-up both salts were formed from the co-deposition of ammonia and the respective organic acid (formic or acetic acid) on an inert substrate (gold) and on amorphous water ice at low temperatures (10 and 120 K) under ultrahigh vacuum conditions. We followed the formation of the salts by infrared spectroscopy and characterized their desorption kinetic properties using the temperature programmed desorption technique. We find the first order kinetic parameters $A = 7.7 \pm 0.6 \times 10^{15}$ s−1 and $E_{bind} = 68.9 \pm 0.1$ kJ mol^{-1} for ammonium formate and $A = 3.0 \pm 0.4 \times 10^{20}$ s^{-1} and $E_{bind} = 83.0 \pm 0.2$ kJ mol^{-1} for ammonium acetate. An experimental evidence is also provided to show that ammonia molecules locked in salts desorb as neutral molecules at temperatures much higher than previously expected that are usually attributed to refractory materials. As a consequence, in star formation regions the ammonia snow line may have a smaller radius than the water snow line. Finally, we discuss how the ratio of NH_3/H_2O content in Solar System bodies can give a hint of where they formed and migrated.

1. S. Viti, M. P. Collings, J. W. Dever *et al.*, *MNRAS*, **354** 1141 (2004)
2. O. Gálvez, B. Maté, V. J. Herrero & R. Escribano, *The Astrophysical Journal*, **724** 53 (2010)
3. P. Vernazza, J Castillo-Rogez, P. Beck, *et al.*, *The Astronomical Journal*, **153** 72 (2017)

Chemical Substructures at 10 au Scales in Protoplanetary Disks: Results from the Molecules with ALMA at Planet-forming Scales (MAPS) Large Program

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Planets form and obtain their compositions in dust- and gas-rich disks around young stars. This process is intimately connected to the spatial arrangement of disk material, but only recently has it become clear that disks are not smooth in either their dust or gas distributions. Dust substructure at 1-to-10 au scales is commonplace, e.g., DSHARP[1], ODISEA[2], but far fewer observations have probed gas substructure at similar scales. To address this, I will present results from the Molecules with ALMA at Planet-forming Scales (MAPS) Large Program, which explores radial and vertical chemical structures at 10 au scales in five disks where dust substructure is detected and planet formation appears to be ongoing. The MAPS observations reveal a striking diversity in the radial morphologies of molecular line emission in protoplanetary disks. Chemical substructures are ubiquitous and extremely varied in their radial locations, widths, and depths. This suggests that planets often form in diverse chemical environments both across disks and even at different radii within the same disk. I will discuss the implications of these findings in the context of interactions between gas and dust substructures in disks and the volatile and organic inventories available to incipient planets. I will also provide some first conclusions about what MAPS is teaching us about the chemistry of planet formation.

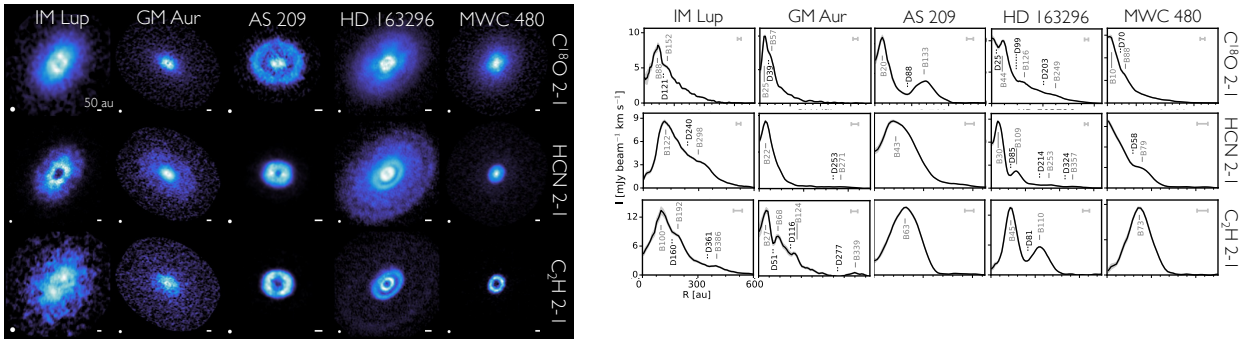

Figure 1: *MAPS reveals >200 chemical substructures in 5 disks across 18 lines, including complex molecules such as HC_3N, CH_3CN, and c-C_3H_2 – only a small sample is shown above.*

1. S. M. Andrews, J. Huang, L. M. Pérez, et al., *ApJL*. **2018**, 869L, 41

2. L. A. Cieza, C. González-Ruilova, A. S. Hales, et al., *MNRAS*. **2021**, 501, 2934

Impact of C/O on the chemistry of PDRs and protoplanetary disks

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Nitriles are key "ingredients" in prebiotic reactions leading to the formation of aminoacids, i.e. life building-blocks. Understanding where and how these molecules form is crucial to determine 1) how universal the seeds of prebiotic chemistry are spread in Space and 2) what type of molecules can be inherited by nascent planets. Complex nitriles, such as HC3N and CH3CN, are observed in a wide variety of astrophysical environments, including at relatively high abundances in photon-dominated regions (PDRs) and the UV exposed atmospheres of planet-forming disks. Mounting evidence suggest that the gas-phase of planet-forming disks is oxygen-poor [e.g., 1, 2]. We recently investigated whether elevated abundances of complex nitriles in UV-irradiated environments could be explained by simple gas-phase PDR chemistry in C-rich environment, i.e. when the elemental C/O ratio is higher than the solar value (~0.5). We find that a C/O ratio higher than ~0.9 can explain the observed nitrile abundances both in PDRs and disk atmospheres, increasing predicted abundances by several orders of magnitude compared to standard C/O assumptions [3]. I will present these new results and show how the C/O ratio appears to be a key variable for complex organic molecule abundances in photon-dominated regions across a wide range of scales.

1. Bergin E. A., Du F., Cleeves L. I., Blake G. A., Schwarz K., Visser R., Zhang K., 2016, ApJ, 831, 101
2. Miotello A., Facchini S., van Dishoeck E. F., Cazzoletti P., Testi L., Williams J. P., Ansdell M., et al., 2019, A&A, 631, A69
3. Le Gal R., Brady M. T., Öberg K. I., Roueff E., Le Petit F., 2019, ApJ, 886, 86

Protostellar shocks as factories of formamide (NH_2CHO), a key prebiotic precursor

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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. This hints at a possible common origin for all living beings existing today on our planet. A promising candidate for this unitary role is formamide (NH_2CHO), a molecule identified as a key precursor of a large variety of organic compounds essential to life[1]. Very interestingly, formamide has been detected in pristine Solar System objects such as comets[2], which leads us to wonder whether these small bodies might have exogenously delivered it in sufficient amounts onto a very young Earth about four billion years ago. A crucial way of addressing this question involves searching for formamide in regions where stars and planets are forming today in our Galaxy, as this can help us understand its chemistry along the different evolutionary phases leading to a star and planetary system like our own.

Formamide has been detected in solar-mass protostars and other interstellar environments[3]. However, its interstellar formation is still a matter of debate: does it form in the gas or on the surface of dust icy mantles? Protostellar shocks are particularly well-suited to answer this, 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 warm chemistry that evolves over time. An illustrative example is the molecular outflow driven by the protostar L1157, which creates several chemically-rich shocks along its path[4]. Interferometric observations of NH_2CHO carried out towards the young shock L1157-B1 with NOEMA (Northern Extended Millimetre Array) as part of the IRAM Large Program SOLIS (Seeds Of Life In Space), combined with astrochemical modelling, revealed that the observed amounts and distribution of NH_2CHO could only be accounted for by gas-phase chemistry[5]. In this contribution, I will present new follow up NOEMA observations of formamide spatially covering the entire southern outflow lobe of L1157, which includes not only B1 but also the older B2 shock, thus allowing us to assess the time evolution of NH_2CHO chemistry. Based on a comparison of the relative abundance of formamide in the two main shocks, and its spatial distribution, I will show how these new observations confirm on more solid grounds that gas-phase synthesis of NH_2CHO indeed appears to be the dominant route in protostellar shocks.

1. Saladino,R., Botta, G., Pino, S. et al. *Chem. Soc. Rev*. **2012**, 41, 5526-5565
2. Biver, N., Bockelée-Morvan, D, Debout, V. et al. *A&A* **2014**, 566, L5
3. López-Sepulcre, A., Balucani, N., Ceccarelli, C. et al. *ACS ESC* **2019**, 3, 2122-2137
4. Bachiller, R. Pérez-Gutiérrez, M., Kumar, M. et al. *A&A* **2001**, 372, 899-912
5. Codella, C., Ceccarelli, C., Caselli, P. et al. *A&A* **2017**, 605, L3

Probing the Chemistry of P-Bearing Molecules in Interstellar Environments and other Extraterrestrial Environments

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Phosphorus is one of the most important elements in biochemistry together with carbon, oxygen, hydrogen and nitrogen. In recent years, phosphorus has been clearly identified in the coma of comet 67P/Churyumov-Gerasimenko[1], while two simple species have been detected in star forming regions, that is, PO and PN[2-5]. If we focus only on solar-type star forming regions, only two detections are available, that is PN and PO toward the shocked region L1157-B1[6] and the Class I protostar B1-b[7]. Phosphorus chemistry in the conditions of the interstellar medium is poorly understood and the interstellar reservoir of this element is strongly debated. The chemistry of interstellar phosphorus and its connections to the P-compounds detected in small bodies of the Solar System remains mostly unexplored and poorly characterized. For this reason, we have undertaken a systematic investigation of possible gas-phase formation routes of simple P-molecules by means of electronic structure calculations, through DFT and CCSD(T) theory, followed by a kinetic analysis using a Rice-Ramsperger-Kassel-Marcus (RRKM) code implemented for this purpose in order to derive the rate coefficients and branching ratios.

1. K. Altwegg, H. Balsiger, et al. , *Sci. Adv*. **2016**,2(5), e1600285
2. V.M. Rivilla, I. Jiménez-Serra, et al., *MNRASL*. **2018**, 475, 1, L30-L34
3. V.M. Rivilla, M.N. Drozdovskaya, *MNRAS*. **2020**, 492(1), 1180-1198
4. V.M Rivilla, F. Fontani, M.T. Beltrán, A. Vasyunin, P. Caselli, J.Martín-Pintado, R. Cesaroni, *ApJ*. **2016**, 826(2), 161
5. V.M Rivilla, F. Fontani, M.T. Beltrán, A. Vasyunin, P. Caselli, J.Martín-Pintado, R. Cesaroni, *IAU Symposium*. **2017**, 13(S332), 409-414
6. B. Lefloch, L. Podio, C. Codella, C. Ceccarelli et al., *MNRAS*. **2016**, 462(4), 3937-3944
7. J.B. Bergner, K.I. Öberg, S. Walker, V.V. Guzmán, T.S. Rice, E.A. Bergin, *ApJL*. **2019**, 884(2), L36

Experimental simulations of Complex Organic Molecule formation in the ISM (with a little help from theory)

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The origin of life on our planet relies on a rich prebiotic chemistry that took place on the surface of the young Earth, potentially triggered by the exogenous delivery of complex organic molecules (COMs). In astrophysics we call COM to any organic molecule with 6 or more atoms[1]. COMs have been detected in comets[2], suggesting that these and other small bodies may be able to deliver material with prebiotic interest to nascent planets.

The origin of these COMs can be traced back to the interstellar medium (ISM) where stars and planetary systems are formed[3]. Therefore, understanding the origin of the molecular complexity in the ISM can help us to better understand the origin of life. In particular, the formation of COMs starts with chemical reactions in the ice mantles detected in dense regions of the ISM, triggered by their energetic processing[4]. These ice mantles can be eventually desorbed to the gas phase (either non-thermally in the cold regions of the ISM, or thermally around forming protostars), and ultimately observed through radio-telescope observations.

Ice chemistry can be studied in the laboratory under astrophysically relevant conditions. In this talk I will review the efforts carried out in the last years to experimentally simulate the formation of COMs in ice samples analog to those detected in the ISM, as well as the insight provided by theoretical models. Interstellar ices are initially formed in the interior of dense molecular clouds by a CO-rich layer deposited on top of a previously grown H_2O-rich layer[5], that contain other simple species (CO_2, NH_3, CH_4) and COM precursors (H_2CO, CH_3OH). These ice mantles can be energetically processed by the cosmic rays that penetrate the interior of dense clouds, and by the subsequently generated secondary UV field. While most studies focus on the chemistry that takes place in the H_2O-rich layer[6], some recent works have studied the induced chemistry in the CO-rich-layer, where the possible presence of H_2 enables the formation of saturated COMs[7]. In quiescent dense clouds, cosmic rays and UV photons can also induce non-thermal desorption of the initial ice components and the chemistry products through different mechanisms[8]. After the onset of star formation, new chemical pathways may become available, including gas-phase reactions upon thermal desorption of the ices[3].

1. E. Herbst, E.F. van Dishoeck, *ARAA* **2009**, 47, 1, 427
2. K. Altwegg, H. Balsiger, A. Bar-Nun, et al., *Sci. Adv.*, **2016**, 2, 5, e1600285
3. K.I. Oberg, E.A. Bergin, *Physics Report*, **2020** 893, 1
4. R.T. Garrod, *A&A*, **2013**, 765, 60
5. A.C.A. Boogert, P.A. Gerakines, D.C.B. Whittet, *ARAA*, **2015**, 53, 541
6. K.I. Oberg, *Chem. Rev.,* **2016**, 116, 17, 9631
7. R. Martin-Domenech, P. Maksyutenko, K.I. Oberg, M. Rajappan, *ApJ*, **2020**, 902, 2, id.116
8. R. Martin-Domenech, G.M. Munoz Caro, G.A. Cruz-Diaz, *A&A*, **2016**, 589, A107

Urea in Astrophysical Environments: IR Spectra and Destruction Cross Sections for Energetic Processing

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Urea (NH_2CONH_2) is a key prebiotic molecule that has been detected in the interstellar medium in the gas phase (1,2) and tentatively in ices (3). In this work, low temperature infrared spectra of urea and urea/H_2O ices, together with infrared band strengths, have been obtained with the goal to guide future searches of this species in ices. Low temperature urea destruction chemistry promoted by UV photons or cosmic rays has also been investigated. Destruction cross sections for energetic processing will be given, following the methodology described in (4).

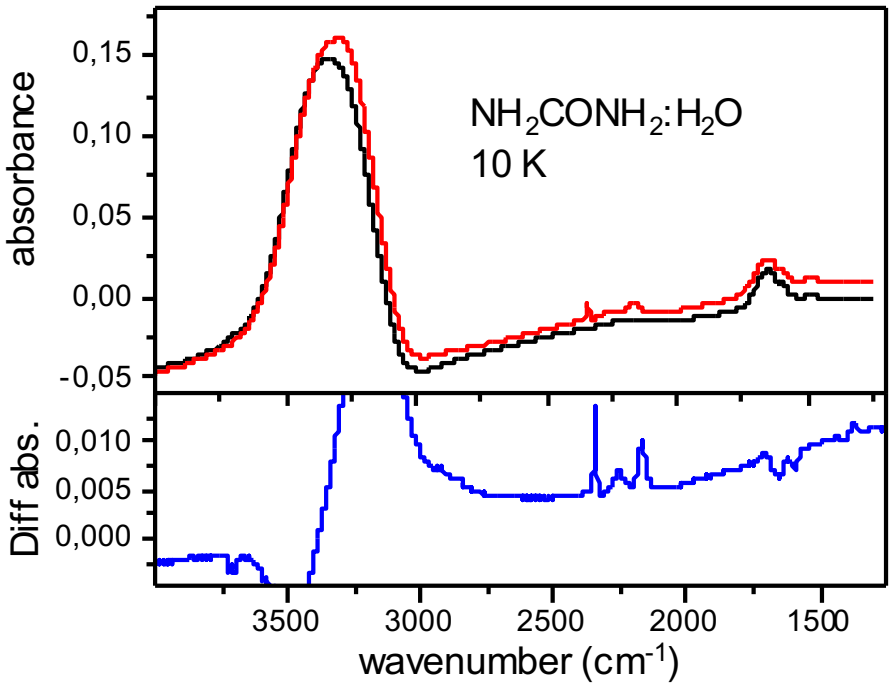

Figure 1: *IR spectra of urea diluted in water ice vapor deposited at 10 K. Black trace: initial spectra. Red trace: final spectra, after 30 min processing with a 5keV e- flux of $2x10^{12}$ cm^{-2} s^{-1}. Blue trace: final-initial difference spectrum,*

1. A. Belloche, R. T. Garrod, H. S. P. Müller, K. M. Menten, I. Medvedev, J. Thomas, and Z. Kisiel, *A&A* **2019**, 628, A10.

2. I. Jimenez-Serra, J. Martín-Pintado, V. M. Rivilla, L. Rodríguez-Almeida, E. R. Alonso, S. Zeng, E. Cocinero, S. Martín, M. Requena-Torres, R. Martín-Domenech, and L. Testi, *Astrobiology* **2020**, 20, 1048- 1066.

3. S.. Raunier, T. Chiavassa, F. Duvernay, F. Borget, J. P. Aycard, E. Dartois, and L. d'Hendecourt, *A&A* **2004**, 416, 165–169.

4. B. Maté, V.J. Herrero, I. Tanarro, V. Timón, H. Carrascosa, G. Muñoz-Caro, C. González-Díaz, and I. Jiménez-Serra, *ApJ* **2021**, 909:123(16pp).

Chemical Inventory of Class I Protostars: A Bridge Between Protostellar Cores and Protoplanetary Disks

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Understanding how molecular complexity varies in Sun-like star forming regions is mandatory to comprehend whether the chemical composition of the protostellar stages is inherited by protoplanetary disks and planets. Class I protostars, with a typical age of 10^5 yr, represent a bridge between Class 0 protostars (10^4 yr), where the bulk of the material that eventually form the protostar is still in the envelope, and the Class II protoplanetary disks (10^6 yr). The importance of the Class I stage has been recently strengthened by ALMA images showing that planet formation occurs already in disks with ages < 1 Myr[1,2].

In this context, and in the framework of the H2020 MSCA ITN Project AstroChemical Origins, we present a chemical census of 4 Class I sources: L1551-IRS5, L1489-IRS (Taurus) and B5-IRS1, L1455-IRS1 (Perseus). We used IRAM-30m observations at 1.3 mm sampling spatial scales of 1500-2500 au. We detect up to 157 lines (depending on the source) due to 27 species: from S-bearing species (OCS, H_2S, CCS, H_2CS), N-bearing (CN, HNCO), C-chains (c-C_3H_2, c-C_3H, CH_3CCH), D-species (CCD, DCN, HDCS, D_2CO, CH_2DOH), molecular ions (N_2D^+, DCO^+) to organic species (H_2CO, H_2CCO, CH_3OH, CH_3CN, CH_3CHO, $HCOOCH_3$). Our observations show a chemical differentiation: (1) All the sources have an extended envelope (up to ~2700 au), characterized by T_{kin} = 15-50K, $n_{H2} \geq 10^3$ cm^{-3}, well traced by narrow lines (1 km/s) due to e.g. C-chains such as c-C_3H_2. (2) L1551-IRS5 has a hot corino (~20 au), with T_{kin} up to 135 K, $n_{H2} \geq 10^8$ cm^{-3}, traced by iCOMs (interstellar complex organic molecules) with broad (3-4 km/s) lines. (3) H_2S and OCS trace the circumbinary disk in L1455-IRS1 and L1551-IRS5. In addition, (4) CH_3OH in the all sources except L1489-IRS shows also a narrow (1 km/s) line component, plausibly due to an extended UV illuminated structure.

CH_3CN, CH_3CHO, $HCOOCH_3$ abundance ratios with respect to CH_3OH as well as D_2CO/H_2CO, CH_2DOH/CH_3OH, and $HDCS/H_2CS$ deuteration ratios are consistent with what has been measured in earlier stages (pre-stellar core, protostars) and more in evolved protoplanetary disks and in Solar System comets.

This suggests that the molecular composition of the latest stages of the Sun-like star forming process is inherited from the earlier phases. The results will be reported in a forthcoming paper[3]. As follow up, we are performing observations on different stages on Solar System scales with interferometry. Once we will have observations on Solar System scale, we will analyze them in light of up-to-date chemical models and binding energies expected for complex species.

1. Sheehan, P. D. & Eisner, J. A. **2017,** *ApJ*, 851, 45 2. Fedele, D., Tazzari, M., Booth, R., et al. **2018**, *A&A*, 610, A24
3. Mercimek, S., Codella, C., Podio L, et al. in preparation

Experimental and Computational Laboratory Astrochemistry – A Personal View

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The application of surface science methodologies to problems in solid state and surface laboratory astrochemistry has seen rapid growth and considerable success over the last two decades. Driven by observational astronomy and the need to explain those observations through simulations capturing the relevant physics and chemistry, early successes of surface science are to be found in the application of temperature-programmed desorption and a little bit of chemical intuition in exploring the trapping and desorption of volatiles in icy films in hot core environments[1,2]; and in the various explorations of molecular hydrogen formation on model grain and ice surfaces[3]. These illustrate the close interaction of laboratory astrochemistry and astrochemical simulation, and within laboratory chemistry of the strong links and complementarity of experimental and computational approaches. This presentation will briefly consider two topics:

(i) Wetting and de-wetting during adsorption on model grain surfaces and specifically how chemical intuition can sometimes let you down; and

(ii) Spontaneous dipole orientation during icy film growth and its astrochemical impact;

and how both experimental and computational laboratory astrochemical understanding contribute (or could contribute) to a deeper understanding of the chemical physics of these systems.

1. M. P. Collings, M. A. Anderson, R. Chen, J. W. Dever, S. Viti, D. A. Williams, M. R. S. McCoustra, *Mon. Not. R. Astron. Soc.* **2004**, 354, 1133-1140.

2. S. Viti, M. P. Collings, J. W. Dever, M. R. S. McCoustra, D. A. Williams, *Mon. Not. R. Astron. Soc.* **2004**, 354, 1141-1145.

3. V. Wakelam, E. Bron, S.Cazaux, F. Dulieu, C. Gry, P. Guillard, E. Habart, L. Hornekær, S. Morisset, G. Nyman, V. Pirronello, S. D. Price, V. Valdivia, G. Vidali, N. Watanabe, *Molec. Astrophys.* 2017, **9**, 1-36.

Neural-Network Assisted Study of H_2 adsorption on solid CO

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H_2 is the most abundant interstellar molecule by a large margin, and, at the temperatures of molecular clouds (10-20 K), it can be present either in the gas phase or on/in interstellar dust grains. The surface of interstellar dust grains at these temperatures is coated with an icy mantle made of different components in different abundances (e.g., H_2O, CO, CO_2). Owing to a small binding between H_2 and interstellar ices, H_2 molecules' fate is to adsorb, diffuse and desorb to/from the grains. The residence time of H_2 molecules on the surface of the grain is pivotal to understand physical processes happening on it, namely nuclear-spin conversion processes or chemical reactivity.[1] In this contribution, we present our recent results on the computational study of the adsorption dynamics of H_2 on solid CO surfaces, a significant component of interstellar ices in the later stages of a molecular cloud lifetime. We employed molecular dynamics simulations driven by neural-network interatomic potentials[2,3] to efficiently sample thousands of adsorption trajectories. Our results[4] show that H_2 weakly binds to the CO surface, limiting the amount of adsorbed H_2 on such a surface.

1. T. Hama and N. Watanabe, *Chem. Rev.* **2013,** 113, 12, 8783-8839
2. V. Zaverkin and J. Kästner, *J. Chem. Theory Comp.* **2020,** 16, 8, 5410-5421
3. G. Molpeceres, V. Zaverkin and J. Kästner, *Mon. Not. Royal. Astron. Soc.* **2020,** 499, 1, 1373-1384
4. G. Molpeceres, V. Zaverkin, N. Watanabe and J. Kästner, *Astron. Astrophys.* **2021,** 648, A84

Complex Organic Molecules from Low- To High-Mass Protostars

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Complex organic molecules are common in both low- and high-mass protostars. Moreover, they are precursors of species that are related to life and hence it is important to study their formation. I will present new results on the complex organic chemistry of the most line-rich sources in the ALMAGAL sample and compare them with those found in a variety of low-mass protostars on Solar System scales.

Our previous studies[1,2] have shown that the abundances of O- and N-bearing species with respect to methanol show remarkable similarities for some species between low- and high-mass sources with large variations in luminosity but not for other species (Fig. 1). However, the number of high-mass sources with such chemistry analysis are only a handful for robust conclusions. Therefore, I will present a more statistical analysis of the chemistry in a high-mass protostellar sample. I will discuss the differences and similarities seen in the abundances of O- and N-bearing species with respect to methanol and deuterated methanol as a function of luminosity. Moreover, I will present a set of radiative transfer envelope plus disk models to explain the dichotomy between line-rich and line-poor sources.

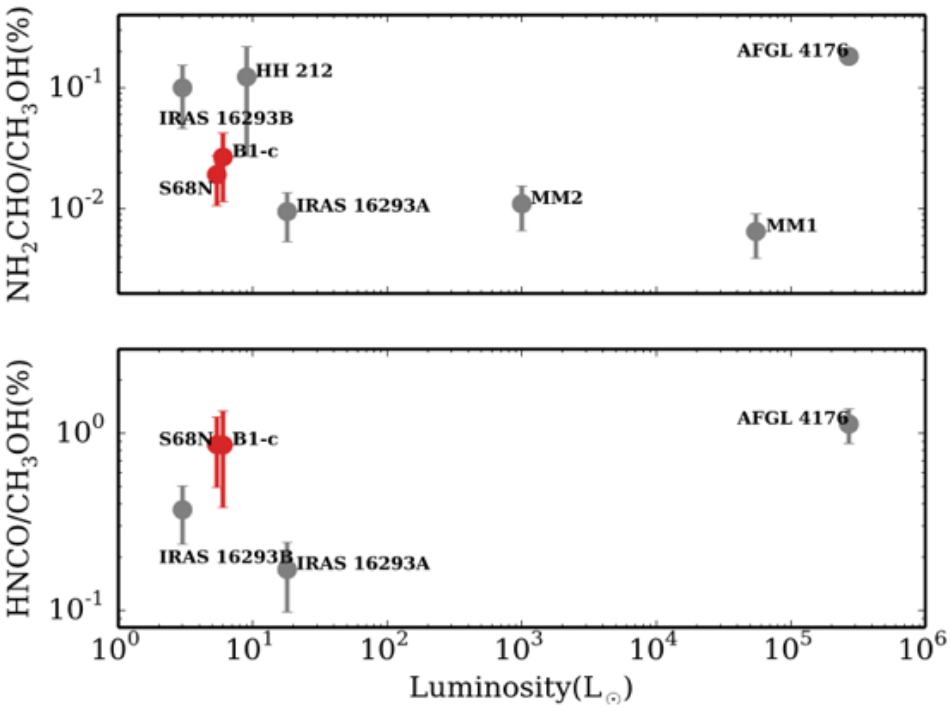

Figure 1: *Column density ratios of NH_2CHO and HNCO with respect to methanol against source luminosity*[1].

1. P. Nazari, et al., *A&A* **2021**, arXiv:2104.03326
2. M. van Gelder et al., *A&A* **2020**, 639, A87

H_2 and HCO· formation on interstellar grains and the fate of reaction energy

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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.[4,5,6,7] Here we report accurate *ab-initio* molecular dynamics simulations aimed at studying the fate of the energy released by two paradigmatic reactions: i) the $H\cdot + H\cdot \rightarrow H_2$ reaction (4.5 eV)[8] and ii) the $H\cdot + CO \rightarrow HCO\cdot$ reaction (1.5 eV),[9] which is the first step of the H addition chain through the methanol (CH_3OH) formation. In both cases, the presence of the ice mantle, acting as third body to absorb the released reaction energy, is mandatory to stabilize the product. Indeed, up to 65% for H_2 and to 90% for HCO· of the kinetic energy liberated by the formation of the new chemical bond is dissipated through the ice. In the case of H_2, its weak interaction with the surface and the large energy kept by the molecule, which can be in a highly vibrational excited state ($v = 6$) ensure the desorption of the species in a relatively short timescale (from 1 ns up to 1000 yr). On the contrary, the HCO· can form three H-bonds with the ice surface and its energy content after the reaction (10–15 kJ mol^{-1}) is not enough to overcome its binding energy (30 kJ mol^{-1}). Therefore, the HCO· is not prone to desorb from the surface, thus allowing the subsequent H addition until the formation of CH_3OH.

1. Ceccarelli, C., Caselli, P., Fontani, F., et al. 2017, ApJ, 850, 176
2. Herbst, E., & van Dishoeck, E. F. 2009, ARA&A, 47, 427
3. D. Hollenbach, E. Salpeter, *J. Chem. Phys.* **1970**, 53, 79-86
4. Garrod, R. T., Wakelam, V., & Herbst, E. 2007, A&A, 467, 1103
5. Duley, W. W., & Williams, D. A. 1993, Mon. Not. R. Astron. Soc., 260, 37
6. Minissale, M., & Dulieu, F. 2014, JChPh, 141, 014304
7. Minissale, M., Dulieu, F., Cazaux, S., & Hocuk, S. 2016, A&A, 585, A24
8. S. Pantaleone, J. Enrique-Romero, C. Ceccarelli, *Astrophys. J.* **2021**, *in press*
9. S. Pantaleone, J. Enrique-Romero, C. Ceccarelli, ApJ, 897, 56

Ice and Gas: Linking Infrared and Millimeter Observations Towards Solar-type Protostars

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The interaction between ice and gas in the Universe is a subtle relationship spanning from the formation of simple molecules to the production of building blocks of planetary systems. There are many unanswered questions about the ice-gas interplay in Solar-type star-forming regions, e.g., what are the exact chemical and physical processes releasing solid-state (ice) molecules into the gas-phase. Such desorption mechanisms are of utmost importance to comprehend some key aspects of star- and planet-formation. Besides enhancing chemical complexity in stellar nurseries, the position at which they occur in protoplanetary disks (snow-lines), influences the composition of forming-planets.

We here introduce a way to address the above questions from an observational perspective: combining infrared (VLT, AKARI, *Spitzer*) and millimeter (SMA, APEX, IRAM 30m) observations of molecular tracers towards Solar-type protostars. Hence, probing the intertwined solid- and gas-phase chemistries to a greater extent than by ice or gas observations alone. We present the results of such combination for the deeply embedded Serpens SVS4 cluster, the multiple proto-stellar system IRAS 05417+0907 in the λ Orionis B35A cloud, and the Coronet cluster in Corona Australis.

We found that ice and gas variations do not follow a predictable trend. Therefore, inferring abundances of solid species from known gas abundances is inaccurate without an extensive knowledge of the underlying physics. Additionally, these comparative studies validate the predicted value for the CH_3OH non-thermal desorption efficiency in low-mass star-forming regions proposed by laboratory experiments and models. Finally, the CH_3OH gas-to-ice ratios show a remarkable similarity, which suggest that the CH_3OH chemistry at play in proto-stellar envelopes in different nearby star-forming regions is relatively independent of variations in the physical conditions.

Linking gas and ice observations will serve as a pathfinder for future JWST and ALMA observations that will provide high sensitivity ice- and gas-maps of complex organics. The combination of infrared and millimeter observations will be an indispensable tool to constrain the routes leading to chemical complexity during the earliest stages of star-formation.

Modeling of the chemical evolution of POx and HPOx (x=2,3) on icy grains

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Phosphorus is one of the fundamental elements involved in many biochemical pathways. On Earth the poorly soluble orthophosphates constitute the main phosphorus reservoir limiting the phosphorus bioavailability compared to less oxidized form of phosphorus (Oxid. States <+3)[1].

Interstellar phosphorus carriers, PO and PN, have been detected in several interstellar objects including star forming regions[2,3], showing a general dominance in the abundance of PO over PN (PO/PN>1)[2]. Currently, the abundance of phosphorus that can be accounted for in the ISM has been observed to be lower than the solar abundance by a factor of 100. [2]

Recent studies on 67P/C-G have shown indication that the phosphorus budget in the comet is depleted only marginally when compared to the solar abundance[4,]. This, along with several evidence suggesting that the chemical composition of 67P/C-G was determined in the pre-stellar phase, validate the hypothesis of grain-sequestered phosphorus species[5]. We found that species such as PO_x and HPO_x (x=2,3) can have very strong binding energies and consequently a semi-refractory behavior which can potentially act as an undetectable sink of phosphorus.

Using the gas-grain chemical code UCLCHEM[6], we explore the formation of phosphorus PO_x and HPO_x (x=2,3) species on icy grains via hydrogenation and oxygenation reactions. We consider Langmuir-Hinshelwood and Eley-Rideal mechanisms of reaction both during the collapse phase and the warmup phase of a molecular cloud. We also evaluate the evolution of the gas-grain fractionation in dependence of the gas temperature to constrain the gas-phase availability of such species. Using the Gaussian 16 suite of software, we determined the binding energies of the POx and HPOx species following the method proposed by Wakelam et Al.[7] and using M06-2X/aug-cc-pVTZ and MP2/cc-pVTZlevel of theory. The binding energies calculated at different level of theory variate for some species. This can lead to a variation in the solid/gas population of these species during cloud evolution. We therefore in parallel compare the effects on the model results in dependence on the calculated binding energy of the species taken in exam.

1. Maciá E. *Chemical Society Reviews*. **2005**;34(8):691-701.

2. Rivilla VM, Fontani FR, Beltrán MT, Vasyunin A, Caselli P, Martín-Pintado J, Cesaroni R. *The Astrophysical Journal.* **2016** Jul 28;826(2):161.

3. Yamaguchi T, Takano S, Sakai N, Sakai T, Liu SY, Su YN, Hirano N, Takakuwa S, Aikawa Y, Nomura H, Yamamoto S. *Publications of the Astronomical Society of Japan.* 2011 Oct 25;63(5):L37-41.

4. Rivilla VM, Drozdovskaya MN, Altwegg K, Caselli P, Beltrán MT, Fontani F, Van der Tak FF, Cesaroni R, Vasyunin A, Rubin M, Lique F. *Monthly Notices of the Royal Astronomical Society.* **2020** Feb;492(1):1180-98.

5. Jiménez-Serra I, Viti S, Quénard D, Holdship J. *The Astrophysical Journal*. **2018** 862(2):128.

6. Holdship J, Viti S, Jiménez-Serra I, Makrymallis A, Priestley F. *The Astronomical Journal*. **2017** 5;154(1):38.

7. Wakelam V, Loison JC, Mereau R, Ruaud M. *Molecular Astrophysics*. **2017** 6:22-35.

The Chemistry of Planet-Forming Disks with ALMA-DOT: towards a comparison with comets to unveil the origin of the Solar System

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What chemical composition planets inherit from their natal environment? Is the chemical composition passed unaltered from the earliest stages of the formation of a star to its disk and then to the planets which assemble in the disk? Or does it reflects chemical processes occurring in the disk and/or during the planet formation process?

The chemical composition of planets and small bodies depends on the location and timescale for their formation and is connected to the spatial distribution and abundance of molecules in the disk. Therefore, a viable way to answer these questions is to compare the chemical content of protoplanetary disks around young Sun-like stars with that of the early Solar System, which is imprinted in comets. With this idea in mind, we initiated the ALMA chemical survey of Disks and Outflows in the Taurus star forming region (ALMA-DOT program). Thanks to the ALMA sensitivity and resolution we obtained images of the disks at ~20-40 au scales, recovering the radial/vertical distribution and abundance of diatomic molecules (CO and CN), S-bearing molecules (CS, SO, SO_2, H_2CS), as well as simple organics (H_2CO and CH_3OH), which are key for the formation of prebiotic compounds.

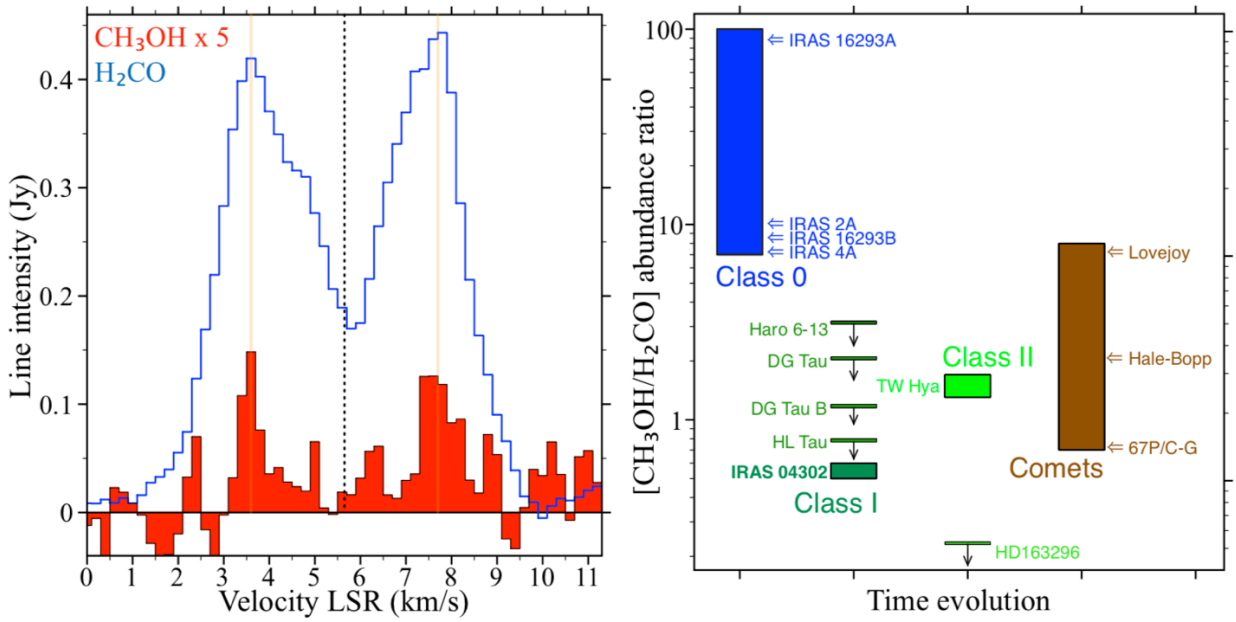

Figure 1. *Left: H_2CO and CH_3OH emission from the IRAS04302 disk. Right: $[CH_3OH]/[H_2CO]$ compared with values for Class 0 hot corinos, other Class I or early Class II disks and comets.*

One of the most intriguing result is the detection of methanol (CH_3OH), one of the key molecule for the formation of complex organic molecules (COMs), in the protoplanetary disk of IRAS04302. The inferred $[CH_3OH]/[H_2CO]$ abundance ratio in the disk is 1-2 orders of magnitude lower than in hot corinos around Class 0 protostars, while it is comparable with that inferred for comet 67P/Churyumov-Gerasimenko. This may be due to chemical evolution, that is, to a chemical reset in the disk with respect to the protostellar stage and/or to the different processes responsible for the release of molecules in the gas phase (thermal desorption in hot corinos and nonthermal desorption in disks). This result is a first step towards reconstructing the chemical path of molecules from protoplanetary disks to comets and planets.

Gas-Phase Reactivity of $[CNH_3]^+$ Ions of Relevance to the Ionosphere of Titan

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The CASSINI mission detected a wide range of N-containing organic ions in the atmosphere of Titan[1], where chemical models[2] predict that their gas-phase reactivity can lead to the formation of increasingly complex species. Here, we present data on the reactivity of two isomers of $[CNH_3]^+$, namely $HCNH_2^+$ and H_2CNH^+, that have been suggested as contributing to the *m/z* 29 peak in the mass spectra of Titan's atmosphere. The experimental data were collected at the SOLEIL synchrotron in Paris[3], using VUV photons to generate our ions while ab initio calculations have also been performed to aid the interpretation of the experimental data.

This data encompasses the reactivity of both isomers with a range of neutrals including saturated; CH_4[4]; and unsaturated; C_2H_2, C_2H_4[5], C_3H_4 (allene), C_3H_4 (propyne) and C_3H_6; hydrocarbons as well as CH_3OH, CO_2, CH_3CN and C_2H_3CN. This allows us to probe the reactivity of both isomers with a range of astrochemically relevant functionalities.

From this, we observe a diverse and different chemistry for the two ions including several pathways involving the formation of either a C-C or a C-N bond, and which can therefore lead to the build-up of chemical complexity in Titan's atmosphere.

1. V. Vuitton, R.V. Yelle and M.J. McEwan, *Icarus*. **2007**, 191, 722-742

2. V. Vuitton et al., *Icacrus*, **2019**, 324, 210-197

3. D. Ascenzi et al., *Frontiers in Chemistry*, **2019**, 7, 537

4. V. Richardson, C. Alcaraz, W. Geppert et al., *Chem. Phys. Lett.* **2021** (In press), https://doi.org/10.1016/j.cplett.2021.138611

5. D. Sundelin, D. Ascenzi, V. Richardson et al., *Chem. Phys Lett.* **2021** (In press), https://doi.org/10.1016/j.cplett.2021.138677

A numerical study of CO kinematics in the CepE-mm Molecular Outflow

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Protostellar jets and outflows are an important agent of star formation feedback, which affects the gas physics and chemistry at all scales, from molecular cloud down to central parental cocoon. Thanks to the advent of 2D/3D chemo-hydrodynamical codes able to model the physical and chemical properties of molecular gas tracers, such as WALKIMYA[1], we are now in position to investigate the complex interaction of jets with the protostellar gas. The CepE-mm protostellar outflow/jet is especially intriguing by the multiple internal shock signatures detected in the CO emission observed with the IRAM interferometer[2] (Fig. 1a) while the jet material is accelerated at hypersonic velocities away from the protostar (Fig. 2b). We will show how comparison between our WALKYMIA simulations and PdBI obervations of the CO emission at arcsec scale allows us to retrieve the 3D history of the mass loss events that shape the CepE-mm system. (Fig. 1b). We will discuss the constraints our simulations place on the ejection process, its interaction with the parental envelope (Fig. 2b), and the CO abundance in the outflow.

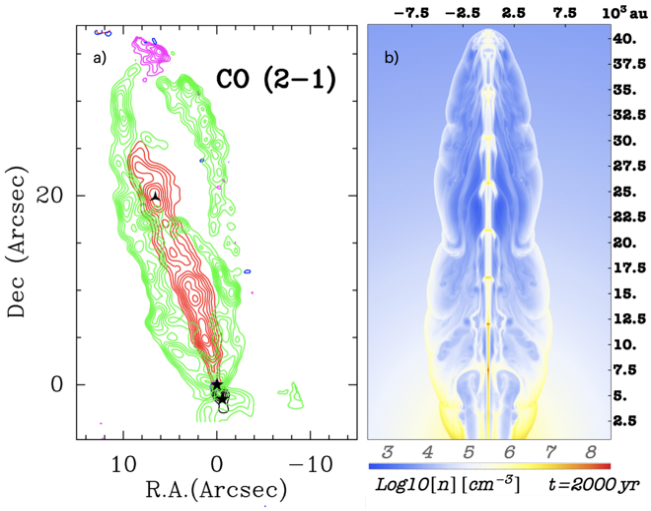

Figure 1: *a) CO emission in the Cep E-mm northern outflow (green) and jet (red) as seen with PdBI. b) Synthetic CO density map from WALKYMIA*

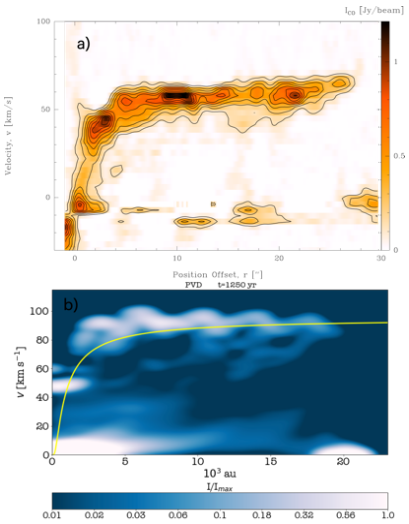

Figure 2: *Position-velocity diagrams of the CO emission obtained from a) PdBI and b) our simulations*

1. Castellanos-Ramírez, A., Rodríguez-González, A., Rivera-Ortíz, P. R., et al. 2018, RMxAA, 54, 409

2. Lefloch, B., Gusdorf, A., Codella, C., et al., 2015, A&A, 581, 4

Prebiotic precursors of nucleic acids, proteins and sugars in Solar-like protostars

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The chemical feedstock of the natal environments of Solar-like protostars (hot corinos) can give us important hints about the chemical heritage that our own Solar System might have received from its birth site. We present in this talk the results of high-angular resolution (< 150 au) ALMA observations towards the archetypical hot corino IRAS 16293-2422 B. We have searched for chemical precursors of key biological macromolecules, such as nucleic acids, proteins and sugars. We reported the first detection of glycolonitrile ($HOCH_2CN$) in the interstellar medium[1], a key intermediate in the formation of nucleic acids. We also reported the first detection towards a Solar-like protostar of its isomer, methyl isocyanate[2] (CH_3NCO), a species involved in the synthesis of proteins. We have also detected towards this hot corino the formyl radical HCO[3], which is the basic building block of many complex organic molecules, and in particular of the simplest sugar glycolaldehye ($HCOCH_2OH$). We have developed several chemical models, including both grain surface and gas-phase chemistry, in order to understand how these key prebiotic precursors can be formed in a hot corino environment.

1. S. Zeng, D. Quénard, I. Jiménez-Serra, J. Martín-Pintado, V. M. Rivilla, L. Testi, R. Martín-Doménech, "First detection of the prebiotic molecule glycolonitrile ($HOCH_2CN$) in the interstellar medium", 2018, Monthly Notices of the Royal Astronomical Society: Letters, Volume 484, Issue 1, p.L43-L48

2. R. Martín-Doménech, V. M. Rivilla, I. Jiménez-Serra, D. Quénard, L. Testi, J. Martín-Pintado, "*Detection of methyl isocyanate (CH_3NCO) in a solar-type protostar*", Monthly Notices of the Royal Astronomical Society, Volume 469, Issue 2, p.2230-2234

3. V. M. Rivilla, M. T, Beltrán, A. Vasyunin, P. Caselli, S. Viti, F. Fontani, F., R. Cesaroni, "First ALMA maps of HCO, an important precursor of complex organic molecules, towards IRAS 16293-2422", Monthly Notices of the Royal Astronomical Society, Volume 483, Issue 1, p.806-82

The first survey of *ortho*-H_2D^+ in high-mass star-forming regions★

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Deuteration has been suggested to be a reliable chemical clock of star-forming regions due to its strong dependence on density and temperature changes during cloud contraction. In particular, the H_3^+ isotopologues (e.g. *ortho*-H_2D^+) seem to act as good proxies of the evolutionary stages of the star formation process. While this has been widely explored in low-mass star-forming regions, in the high-mass counterparts only a few studies have been pursued, and the reliability of deuteration as a chemical clock remains inconclusive.

In this talk, I will present a large sample of *o*-H_2D^+ observations in high-mass star-forming regions and discuss possible empirical correlations with relevant physical quantities to assess its role as a chronometer of star-forming regions through different evolutionary stages.

APEX[1] observations of the ground-state transition of *o*-H_2D^+ were analysed in a large sample of high-mass clumps selected from the ATLASGAL[2] survey at different evolutionary stages. Column densities and beam-averaged abundances of *o*-H_2D^+ with respect to H_2, X(*o*-H_2D^+), were obtained by modelling the spectra under the assumption of local thermodynamic equilibrium. We detect 16 sources in *o*-H_2D^+ and find clear correlations between X(*o*-H_2D^+) and the clump bolometric luminosity and the dust temperature, while only a mild correlation is found with the CO-depletion factor. In addition, we see a correlation with the luminosity-to-mass ratio, which is known to trace the evolution of the star formation process[3]. This would indicate that the deuterated forms of H_3^+ are more abundant in the very early stages of the star formation process and that deuteration is influenced by the time evolution of the clumps.

Our study★ presents the largest sample of *o*-H_2D^+ in star-forming regions to date. The results confirm that the deuteration process is strongly affected by temperature and suggests that *o*-H_2D^+ can be considered a reliable chemical clock during the star formation processes, as proved by its strong temporal dependence.

★. Sabatini, G., Bovino, S., Giannetti, A., et al. **2020**, A&A, 644, A34

1. Güsten, R., Nyman, L. Å., Schilke, P., et al. **2006**, A&A, 454, L13

2. Schuller, F., Menten, K. M., Contreras, Y., et al. **2009**, A&A, 504, 415

3. Molinari, S., Pezzuto, S., Cesaroni, R., et al. **2008**, A&A, 481, 345

Step by Step Strecker Amino Acid Synthesis from Ab Initio Prebiotic Chemistry

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The amino acids synthesis from elementary precursors in abiotic conditions is traditionally described according to the Strecker reaction, thoroughly invoked to justify the observation of amino acids in extraterrestrial samples and their emergence in the primordial Earth. To this day, however, a quantitative microscopic description of the mechanism, thermodynamics, and kinetics of the multistep Strecker reaction is still lacking. In the present work we tackle this study by adopting a state-of-the-art ab initio computational approach, combining an efficient scheme of exploration of the relevant chemical networks with a rigorous determination of the underlying free energy and transition states. We determine the step-by-step chemical pathway from "Strecker precursors" to glycine in solution and calculate the corresponding full free energy landscape. Our results agree well with the scarce available experimental data and complete them, thus providing the first end-to-end study of this complex reaction, a crucial bottleneck for the emergence of life[1].

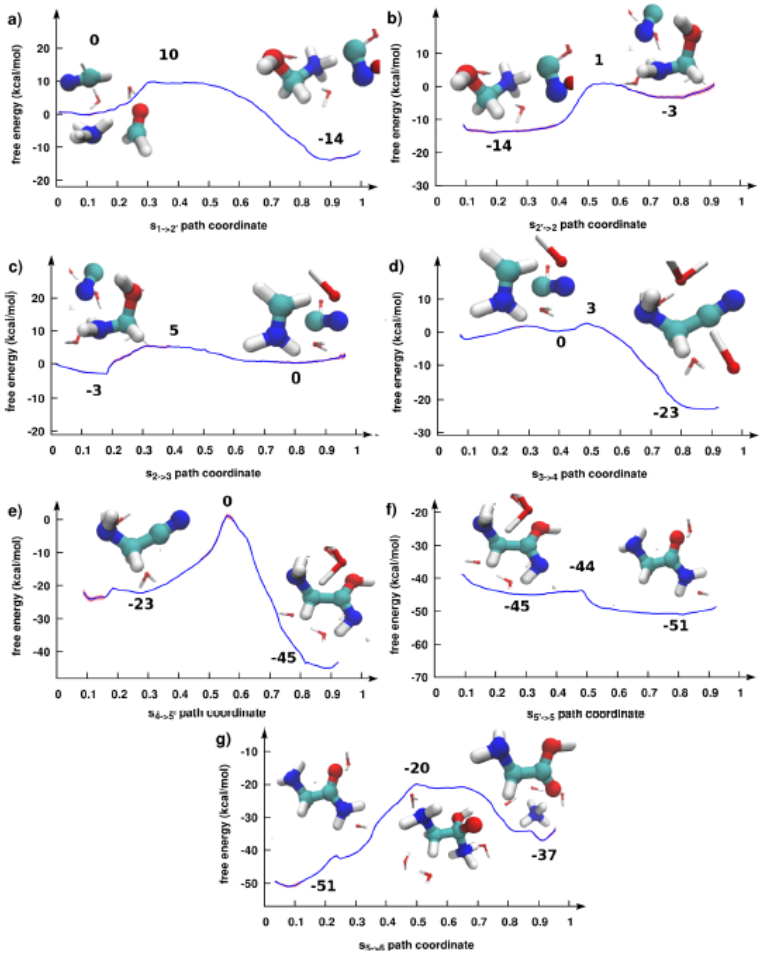

Figure 1: *Umbrella sampling free energy profiles (blue) and error bars (red) for each elementary act. The tetrahedral intermediate (TI5−6) is also shown. Relative free energies are indicated with respect to the Strecker reactants.*

1. T. Magrino, F. Pietrucci, A.M. Saitta, *J. Phys. Chem. Lett.* **2021**, 12, 2630-2637

Reactivity of Gaseous HCN at Amorphous and Crystalline Mg_2SiO_4 Surfaces as Laboratory Models of Interstellar Dust Grains

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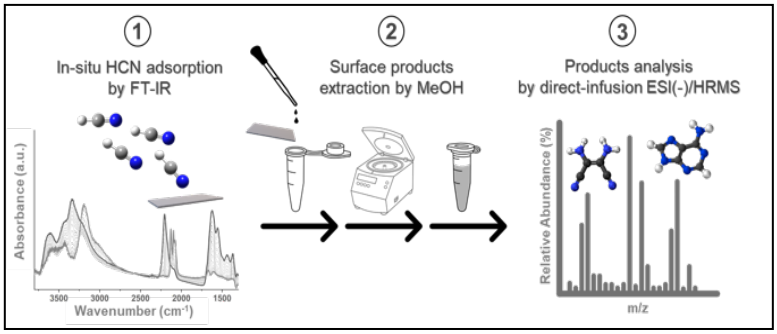
It is well known that the HCN and its derivatives, as key precursors in the formation of several prebiotic biomolecules, are ubiquitous in extraterrestrial environments[1,2].
Furthermore, the recently found complex organic molecules (iCOMs) in the interstellar medium (ISM) have strengthened the idea of an exogeneous origin of the prebiotic matter. As the iCOMs formation involves gas-phase processes and grain-surface reactions, it is assumed that the grain mineral surfaces could play a crucial role as substrates and catalysts[3]. In this exogenous prebiotic scenario, the study of the interaction of gaseous HCN and its derivatives on solids like ice, silica, silicates, and other minerals is relevant for understanding the mechanisms underlying the formation of both iCOMs and more complex nitrogen containing biomonomers like nucleobases.

This work aims to contribute to the above field by studying the adsorption and reactivity of gaseous HCN (produced *in-situ* under controlled and safe conditions) at the surface of two Mg-silicates in amorphous (AMS) and crystalline (forsterite) form, as laboratory models of interstellar dust[4]. Indeed, AMS and forsterite are the major constituents of the dust grain cores in the interstellar medium and in protoplanetary disks, as well as in comets, meteorites, asteroid and protostars. In order to evaluate the role of surface acid-basic sites of such Mg-silicates in HCN reactivity, we have also investigated the HCN 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. The adsorption of HCN from the gas phase and its reactivity were studied by *in-situ* FT-IR as a function of temperature (100-298 K) and the time of contact. To better understand the nature of the reaction products, the methanol-soluble fraction of the adsorbate was analyzed by direct-infusion HR-MS (see schematic workflow on the right).



The results showed that the HCN reactivity occurred only at the surface of MgO and Mg-silicates suggesting that the Lewis surface basicity due to the coordinatively unsaturated O^{2-} sites (absent in SiO_2) could play a key role in the process. This represents an important step forward in HCN reactivity investigation because highlights that also in mild experimental conditions (low HCN equilibrium pressure, low temperature, absence of external energy sources like UV irradiation or electrical discharges) the HCN is able to form several N-heterocyclic compounds including adenine nucleobase.

1. L. M. Ziurys, B. E. Turner, *Astrophys. J.* **1986**, 302, L31-6.
2. C. N. Matthews, R. D. Minard, *Faraday Discuss*. **2006**, 133, 393-401, discussion 427-52.
3. E. Herbst, E. F. van Dishoeck, *Annu. Rev. Astron. Astrophys.* **2009**, 47 (1), 427-480.
4. M. Signorile, L. Zamirri, A. Tsuchiyama, P. Ugliengo, F. Bonino, G. Martra, *ACS Earth Space Chem.* **2020**, 4 (3), 345-354.

Molecules in Protostellar Jets: Lessons from CepE-mm

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It has become increasingly clear in recent years that protostellar jets play an important role in the chemical evolution of star and planet forming systems. These jets interact with the circumstellar envelope through shocks, and drive rich chemistry in the material which ultimately feeds the nascent protostar. Whereas shock-driven chemistry is now investigated in detail with major (sub)mm interferometers ALMA and NOEMA, the jet composition and the origin of the molecular material (most often simple O-bearing species) remain a major enigma of star formation studies. The mystery thickened with the case of the young intermediate-mass protostellar source CepE-mm[2], which exhibits a composition unlike any other jet.

We will present the results of our deep molecular line survey of the CepE-mm jet in the framework of the Large Program SOLIS[1]. Highly anomalous chemical composition is detected in the jet with, for the first time, the presence of organic molecules such as CH_3OH and H_2CO, and other species like CS and HCO^+. A complex spatial differentiation is observed between species along the jet length. Thanks to hydrodynamical simulations of the CepE-mm outflow/jet with WALKYMIA-2D[4], we will discuss the origin of such differentiation and will show how the jet dynamics and chemistry are tightly linked, shedding new light on the origin of molecules in jets.

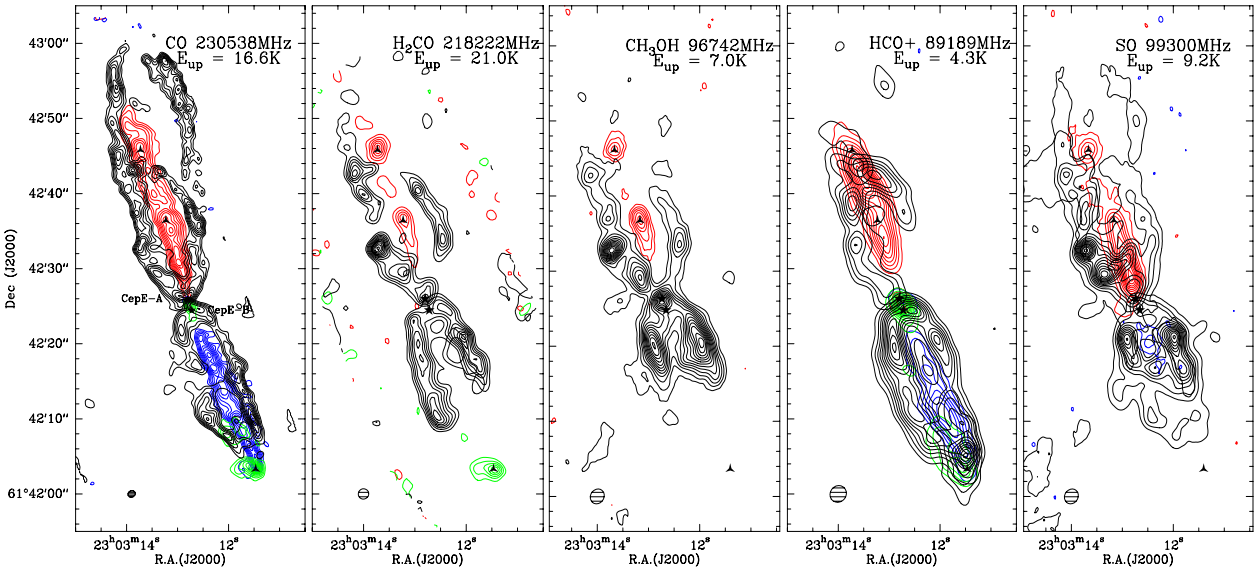

Figure 1: *Velocity-integrated emission maps of some molecular species detected along in the CepE-mm jet (from left to right): CO, H_2CO, CH_3OH, HCO^+ and SO. The two lobes of the jet are drawn by red and blue contours, the emission of the outflow cavities is superposed in black, while the green contours represent the emission from the terminal bow shock HH 377.*

1. Ceccarelli, C. et al. **2017**, ApJ, 850, 176; **2**. Ospina-Zamudio, J. et al. **2018**, A&A, 618, A145;
3. Ospina-Zamudio, J., et al. **2019**, MNRAS, 490, 2679; **4.** Castellanos-Ramírez, A., et al. **2018**, RMxAA, 54, 409.

What do pristine Solar System materials tell us about the origin and early evolution of the Solar System?

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The Solar System was born 4.567 billion years ago from the Sun's parent molecular cloud. The earliest epoch of the Solar System formation is expected to be recorded in pristine Solar System bodies. Recent Solar-System exploration missions have revealed chemistry of a pristine comet (Rosetta: 67P/Churyumov-Gerasimenko)[1], explored carbonaceous-type asteroids (Hayabusa2: Ryugu; OSIRIS-REx: Bennu)[2,3], and returned pristine asteroidal samples (Fig. 1)[4]. The detailed analysis of remote sensing data, obtained from proximity observation of small bodies, and returned primordial samples will provide us a unique opportunity to explore the origin and early evolution of the Solar System. Some recent progresses of Solar-System small body explorations and extraterrestrial sample analysis will be reviewed in the presentation.

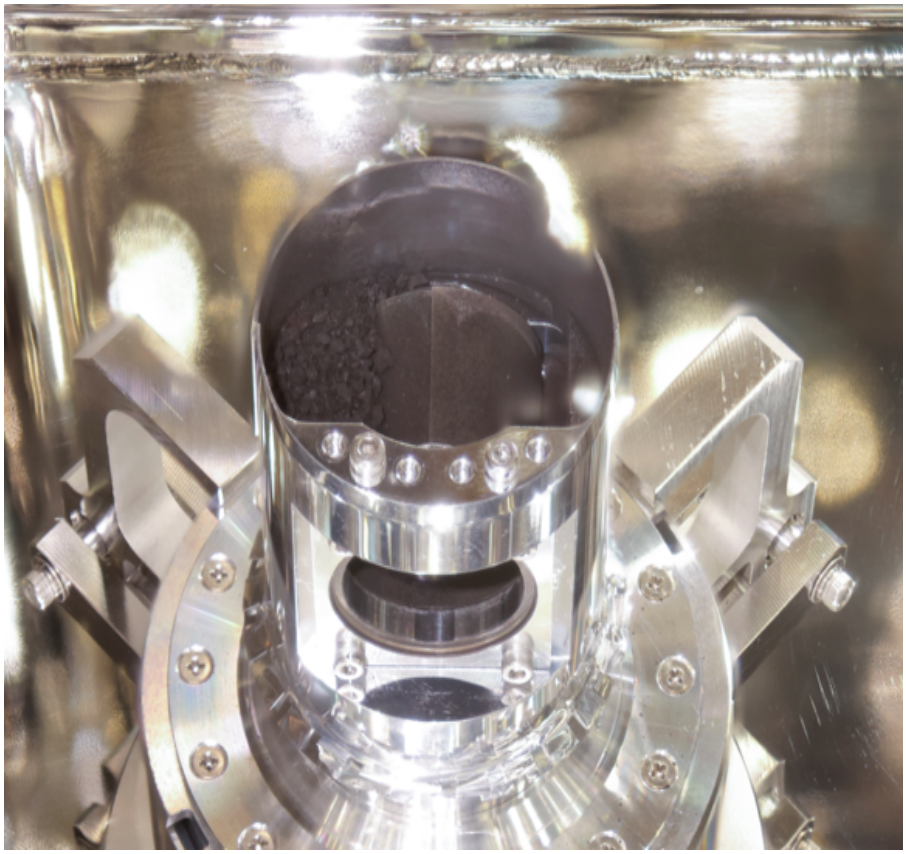

Figure 1: *Dark surface samples retuned from C-type asteroid (162173) Ryugu*

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1. K. Altwegg et al., *Science* **2008**, 347, 1261952
2. S. Watanabe et al., *Science* **2019,** 364, 268–272
3. S. Sugita et al., *Science* **2019,** 364, eaaw0422
4. S. Tachibana et al., *Lunar Planet Sci.* **2021,** 52, #1289

The Effects of Episodic Accretion on the Chemistry of the Protostellar Discs and Envelopes

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Protostellar cores exhibit a rich and diverse chemistry, and it is also known that the embedded protostars commonly experience phases of episodic, increased accretion. To connect these facts and to understand this complex physical and chemical system, one needs to couple dynamics to chemical modeling. We present a study of the spatio-temporal evolution of complex organic molecules in an episodic accretion scenario, with the aim of understanding the processes involved in the early phases of star formation and the coeval chemical evolution. We carry out smoothed particle hydrodynamics (SPH) simulations of low-mass star formation in collapsing, turbulent prestellar cores. The included sub-grid episodic accretion model efficiently heats the proto-stellar accretion disk and drives episodic outflows (Rohde et al. 2021[1]) .We extract the density and temperature evolution of a subset of SPH particles and apply the astro-chemistry code Saptarsy (Choudhury et al. 2015[2]). Saptarsy is a rate-equation-based 1D astro-chemical code which includes gas-phase reactions, gas-grain interactions and surface chemistry, as well as multilayered dust chemistry. We investigate the time evolution of numerous gas phase tracers and look at the effects of the episodic flares on the chemistry surrounding the proto-stars. The episodic accretion flares produce an abrupt temperature change with lifetimes of a few decades. We find that different species react a variety of ways, a group of species are elevated in the interior eg. CH3OH abundance changes by 3 orders of magnitude within 1500 AU, whereas some others like HCO+ get destroyed, decreasing abundance by 2 orders of magnitude within 1000 AU. The response time to the flares varies considerably and some molecules are not affected at all. This work suggests that one might be able to use a set of different molecules to build a chemical clock based on the episodicity in the chemical response to the accretion flares.

1. Rohde, P. F., S. Walch, S. D. Clarke, D. Seifried, A. P. Whitworth, and A. Klepitko. "The impact of episodic outflow feedback on stellar multiplicity and the star formation efficiency." Monthly Notices of the Royal Astronomical Society 500, no. 3 (2021): 3594-3612.

2. Choudhury, Rumpa, Peter Schilke, Gwendoline Stéphan, E. Bergin, Thomas Möller, Anika Schmiedeke, and Alexander Zernickel. "Evolution of complex organic molecules in hot molecular cores-Synthetic spectra at (sub-) mm wavebands." Astronomy & Astrophysics 575 (2015): A68.

A New Approach to Compute Accurate Binding Energy Distribution of Complex Organic Molecules at Ice Interstellar Grain Models: the Case of NH_3

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In the denser ($\geq 10^4$ cm^{-3}) and colder ($\leq$20 K) regions of the interstellar medium (ISM), sub-micron sized dust grains are covered by several layers of H_2O-dominated ices[1]. The composition and thickness of these ices is governed by whether molecules and atoms remain glued to the grain surfaces or not and whether they can move on the surfaces and scan them, so to meet other species and react. On the other hand, in warmer regions, these interstellar ices can (partially) sublimate and enriched the gas of its components. The ice-gas interaction is, therefore, a hugely important process that determines the chemical composition of the ISM. The basic quantity that rules all these processes is the binding energy (BE) of the species to the interstellar ice surface. It is thus not an exaggeration to affirm that the BE of interstellar atoms and molecules is a small quantity with a huge impact. So far, with very few exceptions, astrochemical models have assumed single values for each species BE. In this work, we present a new and robust computational strategy to evaluate BEs by theoretical computations on a novel amorphous solid water (ASW) cluster[2]. This cluster exhibits a large number of adsorption sites where NH_3 (our test molecules) can be adsorbed. The BEs are computed through the ONIOM[3] approach using a QM:QM layer envisaging xTB-GFN2[4] as the low method and DLNPO-CCSD(T)[5] as the high level method. The generality of xTB-GFN2 as a low-level method allows to treat a large variety of interstellar species, at variance with the adoption of *ad hoc* force fields as currently done in the literature. As a first study and astrochemically important case, we applied this new methodology, to derive the BE distribution of ammonia, computed on about 160 different adsorptions shown in the right figure. Machine learning clustering analysis is performed and further the two clusters found were fitted by Maxwell-Boltzmann distributions, which reflect the different nature of the possible bonds of NH_3 on ASW. Particularly important is the low-energy end of the BE distribution, which has an unexpected impact on some astrochemical situations, like protoplanetary disks.

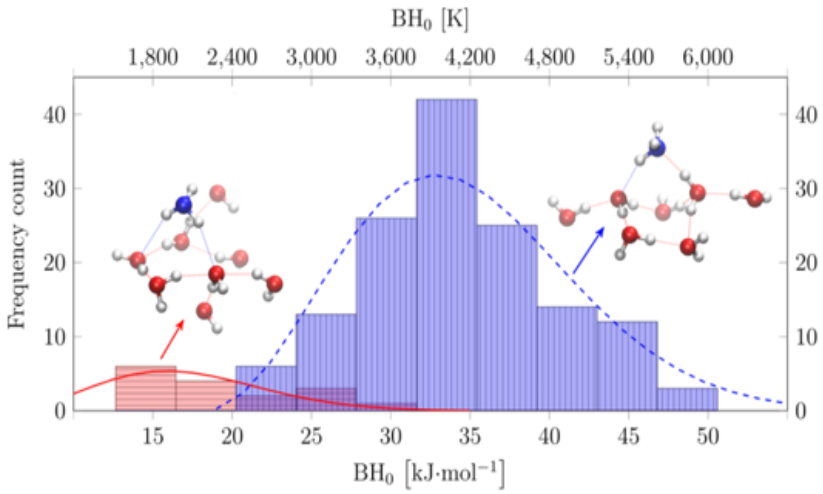

Figure 1: NH_3 ZPE corrected BE distribution

1. A. Boogert, et al., *ARRA* **2015**, 53, 541
2. A. Germain, et al., *to be submitted*
3. S. Dapprich, et al., *J. Mol. Struct.* **1999**, 462, 1-21
4. C. Bannwarth, et al., *J. Chem. Theory & Comp.* **2019**, 15(3), 1652-1671
5. Y. Guo, et al., *J. Chem. Phys.* **2018**, 148, 011101

Which Molecule Traces What?
Chemical Diagnostics of Protostellar Sources Revealed with ALMA.

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The physical and chemical conditions in Class 0/I protostars are fundamental in unlocking the protostellar accretion process and its impact on planet formation. We use a suite of Atacama Large Millimeter/submillimeter Array (ALMA) datasets in Band 6 (1 mm), Band 5 (1.8 mm) and Band 3 (3 mm) at spatial resolutions 0.5 – 3 arcsec for 16 protostellar sources. This is an effort to pinpoint chemical tracers to the physical components of the young protostellar systems at the Solar System scales (50 au). Cold gas tracers like $C^{18}O$, DCO^+ and $N2D^+$, associated with the freeze-out of CO are tracing quiescent envelope material. Shock tracers such as SiO and SO are seen in the outflow; additionally, ice-mantle products released with the shock are also detected. SiO, SO and occasionally H_2CO are detected in the high-velocity molecular jet. The cavity walls show tracers of UV-irradiation such as hydrocarbons C_2H and c-C_3H_2 as well as CN. The hot inner envelope, apart from complex organic molecules (COMs), also presents compact emission from small molecules like H_2S, SO, OCS and $H^{13}CN$, most likely related to thermal ice sublimation. Fig. 1 presents a summary of this work, showing a set of best chemical tracers for different physical components. I will put these results in the context of the upcoming James Webb Space Telescope (JWST). From our targets, 12 will be targeted by JWST with MIRI and NIRSpec observations. ALMA provides a kinematic map of components for which JWST will deliver the sub-arcsecond observations in near- and mid-infrared for the first time.

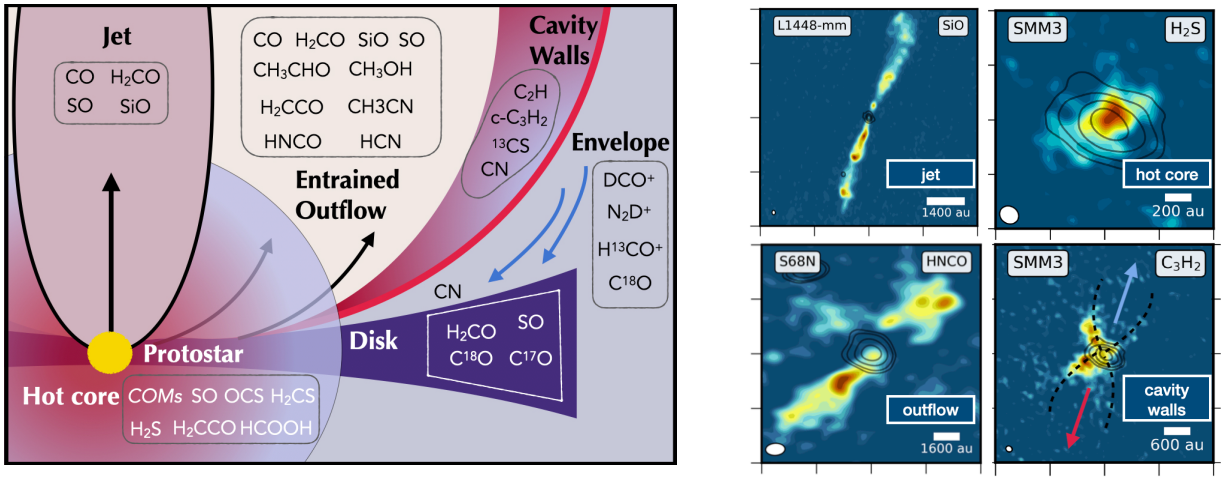

Figure 1: *Left: Summary cartoon of the key molecular tracers of different components, exclusive to molecules presented in this work. Right: Maps of different physical components mapped with different molecules*

Modeling Accretion Shocks at the Disk-Envelope Interface: Sulfur Chemistry

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A major question in the star-formation process is to what extent the chemical composition is preserved from cloud to disk ('inheritance'), or whether it will be modified en route ('reset') due to a strong accretion shock as the material enters the disk (see Figure 1). Since planet formation is thought to start early, in the disk of an embedded protostellar system, the presence of an accretion shock might alter the composition of the material accreted by young forming planets.

Recent high-angular resolution ALMA observations[1,2,3] hint at shocks near the disk-envelope interface toward the youngest protostellar systems via the detection of warm SO and SO_2. However, the interpretation of these millimeter data is ambiguous, since the emission could also be related to outflow activity and heating by the protostar. Here, we will introduce a grid of low-velocity (< 10 km s^{-1}) *J*-type shock models in high density (10^{5-8} cm^{-3}) conditions computed using the Paris-Durham shock code[4] to investigate whether the abundance of SO and SO_2 increases in such shocks and if so, how they can help us to constrain the strength of the shock.

In lower-velocity (~ 3 km s^{-1}) shocks, hydrocarbons such as CH_4 and H_2CO play a role in forming SO through reactions with S^+. In higher velocity (> 4 km s^{-1}) shocks, both SO and SO_2 are formed through reactions of OH and atomic S. The strength of the UV radiation field is crucial for SO and in particular SO_2 formation through the photodissociation of H_2O. Thermal desorption of SO and SO_2 ice is only relevant in high-velocity (> 5 km s^{-1}) shocks at high densities (> 10^7 cm^{-3}). The abundances of SO and SO_2 thus provide unique constraints on the shock strength (i.e., velocity, density) and so on the amount of reprocessing experienced by material entering the disk. Moreover, combination with future JWST observations on e.g., H_2 and H_2O will provide an excellent synergy with current ALMA observations.

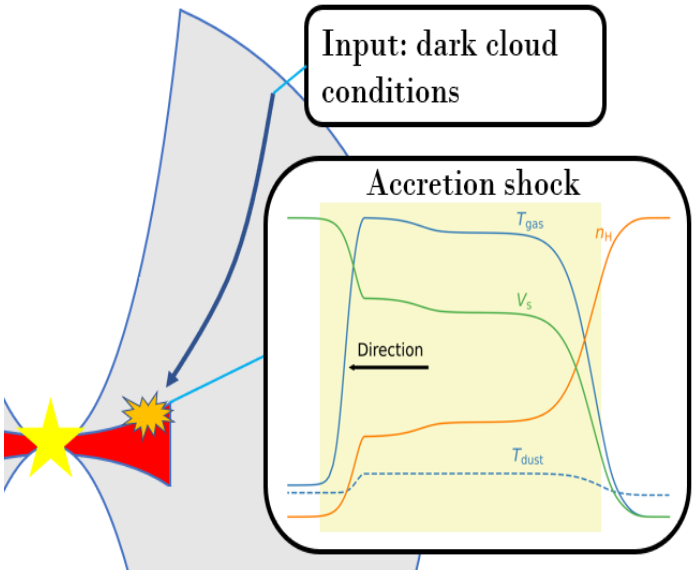

Figure 1: Physical structure of a protostellar envelope. Starting with dark cloud conditions, an accretion shock model is calculated.

1. Sakai, N. et al. 2014, Nature, 507, 78
2. Oya, Y. et al. 2019, ApJ, 881, 112
3. Artur de la Villarmois, E. et al. 2019, A&A, 626, A71
4. Godard, B. Et al. 2019, A&A, 622, A100

Gas-phase Formation of Acetaldehyde: Review and New Theoretical Computations

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The question of the formation of Complex Organic Molecules (*COMs*) in ISM is a main issue in the field of prebiotic chemistry. In this context, acetaldehyde is a particularly important species, being a possible precursor for several carbohydrates[1,2] and acrolein (a crucial intermediate in the prebiotic synthesis of various amino acids)[3]. It can also be considered as a condensation agent in the prebiotic formation of deoxyribonucleosides[4], a major component of DNA. Moreover, its key role in ISM appears to be also remarkable since it is one of the first[5] and most widely detected species[6]. The question of its formation is therefore of a major interest regarding astrochemical models, even though there is still not a consensus on how this molecule is formed. It could be either the product of the chemistry occurring on the grain ice surfaces or synthesized in the gas phase - or both.

In this contribution, we will focus on the gas-phase formation routes that have been proposed in the literature. Using a computational strategy integrating state-of-the-art electronic structure calculations and kinetic calculations, we provide a completely validated network of gas-phase reactions that form acetaldehyde and that can therefore be used in astrochemical models.

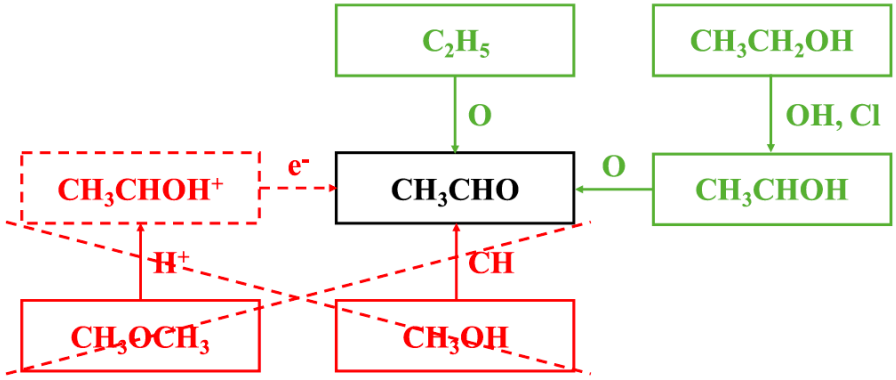

Figure 1: *Considered reactions*[8]

1. S. Pizzarello, A. L. Weber, *Science*, **2004**, 303, 1151
2. A. Cordova, I. Ibrahem, J. Casas, H. Sunden, M. Engqvist, E. Reyes, *Chem. Eur. J.*, **2005**, 11, 4772
3. H. J. Cleaves II, *Monatshefte fur Chemie / Chem. Mon.*, **2003**, 134, 585
4. J. S. Teichert, F. M. Kruse, O. Trapp, *Angew. Chem. Int. Ed.*, **2019**, 58, 9944
5. C. A. Gottlieb, in Gordon M. A., Snyder L. E. eds, Molecules in the Galactic Environment. *Wiley-Interscience*, **1973**, p. 181
6. E. Bianchi et al., *MNRAS*, **2019**, 483, 1850
7. M. De Simone et al., *A&A*, **2020**, 640, A75
8. F. Vazart, C. Ceccarelli, N. Balucani, E. Bianchi, D. Skouteris, *MNRAS*, **2020**, 499, 5547

A New Platform for Generating, Storing and Accessing High Quality Quantum Chemical Data of Molecular Binding Energies on Interstellar Icy Grain Surfaces

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Chemical and physical processes on icy-grains surfaces are a key component for astrochemical models as these ices can act as a molecular sink and as catalysts for reactions of interstellar molecules. In this work we present a new database of molecular binding energy distributions that are generated using a thorough electronic structure protocol to ensure the creation of high quality and reliable data.

The ice models are generated through *ab initio* molecular dynamics while the binding energy data is obtained using density functional theory after extensive benchmarking on small ice clusters using correlated coupled cluster methods[2]. The database to generate and store the data is built on the QCArchive[1] framework that standardizes the generation of quantum chemical data and makes it highly accessible for any researcher in the field of quantum chemistry and computational astrochemistry modeling. Furthermore, the binding energy distributions stored in the database can be used as a starting point for the study of diffusion processes and chemical reactions.

1. G. Bovolenta, S. Bovino, E. Vöhringer-Martinez, D. A. Saez, T. Grassi, S. Vogt-Geisse, *Molecular Astrophysics*, **2020**, 21, 100095

2. D. G. A. Smith, D. Altarawy, L. A. Burns, M. Welborn, L. N. Naden, L. Ward, S. Ellis, B. P. Pritchard, and T. D. Crawford, *WIREs Computational Molecular Science*, **2021**, 11, 2

X-ray Flare Driven Chemical Evolution in Planet Forming Regions

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Chemical evolution in planet forming regions, or protoplanetary disks, is largely driven by radiation from the young central star. Solar-mass pre-main sequence stars, or T-Tauri stars, are considered X-ray bright[1], where the high X-ray luminosity is able to penetrate the surrounding disk and drive chemistry via ionization of H_2 [2,3]. However, T-Tauri stars, are also considered highly variable in the X-ray regime due to frequent magnetic reconnection events on the stellar surface[4]. These X-ray 'flares' are known to increase X-ray ionization rates in the surrounding protoplanetary disk, thus driving new flare driven chemistry[5].

In this contribution, we discuss modeled X-ray flare driven chemical evolution in a protoplanetary disk. We specifically highlight the evolution of biologically relevant species, such as organic species and sulphur bearing species. Individual X-ray flares most strongly affect small gas-phase cations, where a single flare can temporarily enhance the abundance of species such as HCO^+, CH_3^+, and C^+. Over the course of the 500 year model, the stochastic enhancement of these species drives a new chemical steady state (Figure 1). Some carbon chains and organosulphides reach a new chemical 'equilibrium' in the disk, suggesting that X-ray flares contribute to the global chemical evolution in planet forming regions.

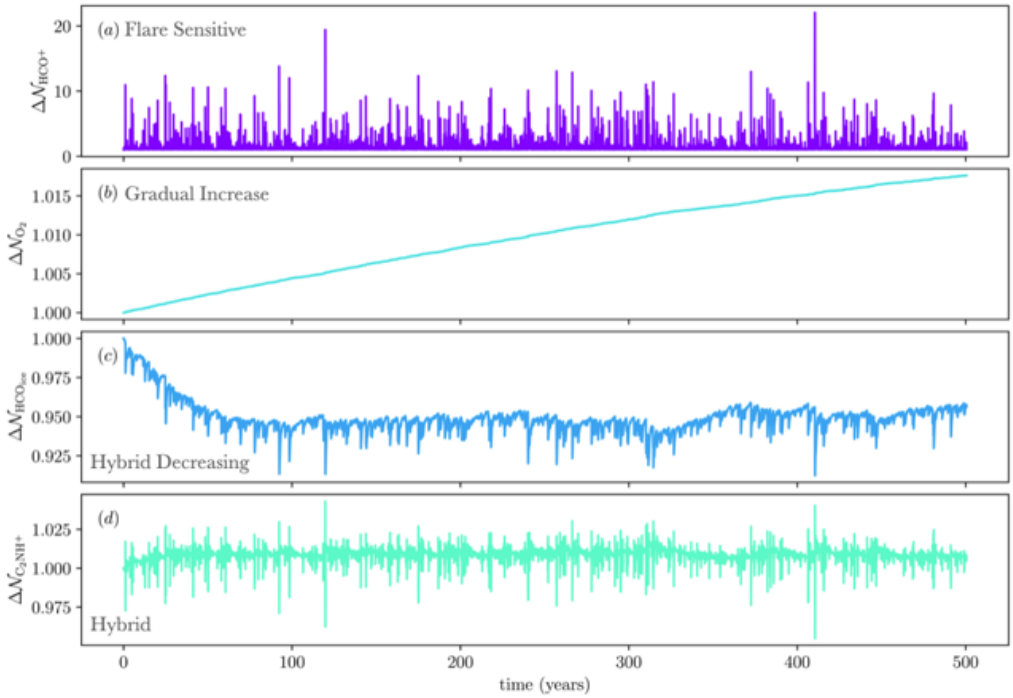

Figure 1*: Example types of changes seen in the disk integrated abundance (w.r.t. H) of different molecular species relative to a model without X-ray flares. Note the variety of chemical responses.*

1 Wolk, S, J., Harnden, Jr., F. R., Flaccomio, E., et al. **2005**, ApJS, 160, 423, doi: 10.1086/432099
2 Glassgold, A. E., Najita, J., & Idea, J. **1997**, ApJ, 480, 344, doi: 10.1086/303952
3. Maloney, P. R., Hollenback, D. J., & Tielens, A. G. G. M. **1996**, ApJ, 466, 561, doi: 10.1086/177532
4 Gudel, M. **2004,** A&A Rv, 12, 71, doi: 10.1007/s00159-004-0023-2
5 Waggoner, A. R., & Cleeves, L. I. **2019**, ApJm 883, 197, doi: 10.3847/1538-4357/ab3d38

Interstellar icy mantle formation in molecular clouds

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Molecular Clouds (MCs) are the birthplace of stars and planets, and the first step towards their molecular complexity. Indeed, in MCs the interstellar submicron sized dust grains become covered by dirty icy mantles, whose water is the major component followed by CO, CO_2, CH_3OH and NH_3, among other much less abundant molecules. Past observations and modelling suggest that the precise composition of the grain icy mantles depends on the physical conditions of the considered MC as well as its history. The imminent launch of the James Webb Space Telescope (JWST: Gardner et al. 2006), with its unprecedented high spectral resolution and sensitivity, will allow us to obtain a breakthrough in the grain icy mantle composition of a variety of quiescent MCs and probably address the origin of this variety.

In fact, the formation of MCs has been a subject of debate for decades. Observations and Hydrodynamical (HD) simulations has shown us that there are various paths to forming a MC from the initial status, that is believed to be the Cold Neutral Medium (CNM), i.e. cold (~100 K) clouds of neutral hydrogen. In this work, we aim to exploit the dependence of the grain icy mantles on the MC history coupled with the available observations to constraint the MC formation process and provide a grid of model predictions for the comparison with the future JWST ones.

We present the gas-grain model GRAINOBLE+, the upgraded version of GRAINOBLE (Taquet et al. 2012), to model the transition from the CNM to MC and predict gaseous and icy chemical composition in MCs. We included the latest calculations of the binding and diffusion energies (e.g. Ferrero et al. 2020; He et al. 2018), and updated gas-phase and grain-surface reaction networks (see details in Vazart et al. 2020 and Enrique-Romero et al. 2019). In this presentation, we compare the new GRAINOBLE+ predictions with the observations towards the Taurus MC. We run several models with various initial parameters and CNM-MC transition histories, from static to evolving physical conditions based on HD simulations (e.g. Zamora-Avilés et al. 2014).

[1] Gardner, J. P., Mather, J. C., Clampin, M., et al. 2006, SSRv, 123, 485, doi: 10.1007/s11214-006-8315-7
[2] Taquet, V., Ceccarelli, C., & Kahane, C. 2012, A&A, 538, A42, doi: 10.1051/0004-6361/201117802
[3] Ferrero, S., Zamirri, L., Ceccarelli, C., et al. 2020, ApJ, 904, 11, doi: 10.3847/1538-4357/abb953
[4] He, J., Emtiaz, S., & Vidali, G. 2018, ApJ, 863, 156, doi: 10.3847/1538-4357/aad227
[5] Enrique-Romero, J., Rimola, A., Ceccarelli, C., et al. 2019, ACS Earth and Space Chemistry
[6] Vazart, F., Ceccarelli, C., Balucani, N., Bianchi, E., & Skouteris, D. 2020, MNRAS, 499, 5547, doi: 10.1093/mnras/staa3060
[7] Zamora-Avilés, M., & Vázquez-Semadeni, E. 2014, ApJ, 793, 84, doi: 10.1088/0004-637X/793/2/84

A Hot Gravitationally Unstable Disk as the Origin of the Class 0 Hot Corino IRAS 16293-2422 B

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Deeply embedded protostars are actively fed from their surrounding envelopes through their protostellar disk. The physical and chemical structure of such early disks might be different from that of more evolved sources due to the active accretion. In this contribution, we present 1.3 and 3 mm ALMA continuum observations at resolutions of 6.5 au and 12 au, respectively, towards the Class 0 protostar IRAS 16293-2422 B, the very first source identified as a hot corino. The resolved brightness temperatures appear remarkably high, with T_b >100 K within ~30 au and a peak value over 400 K at 3 mm. Both wavelengths show a lopsided spatial distribution of the emission with a spectral index lower than 2 in the central ~20 au region. We compared these observations with a series of radiative transfer calculations and synthetic observations of protostellar disk models formed by the collapse of a dense core. We find that a massive young gravitationally unstable disk model can reproduce the high observed T_b values and resolved spectral index. The gas kinematics within this disk model (e.g., shocks and compressional heating) play a more significant role in heating the disk than the protostellar radiation. The structures arising in a gravitationally unstable disk could also explain the observed asymmetry. Our results suggest that a young self-gravitating disk could be at the origin of a hot corino and that its high temperatures are responsible for releasing volatile species back in the gas phase, providing an explanation for the highly rich chemistry found in this source.

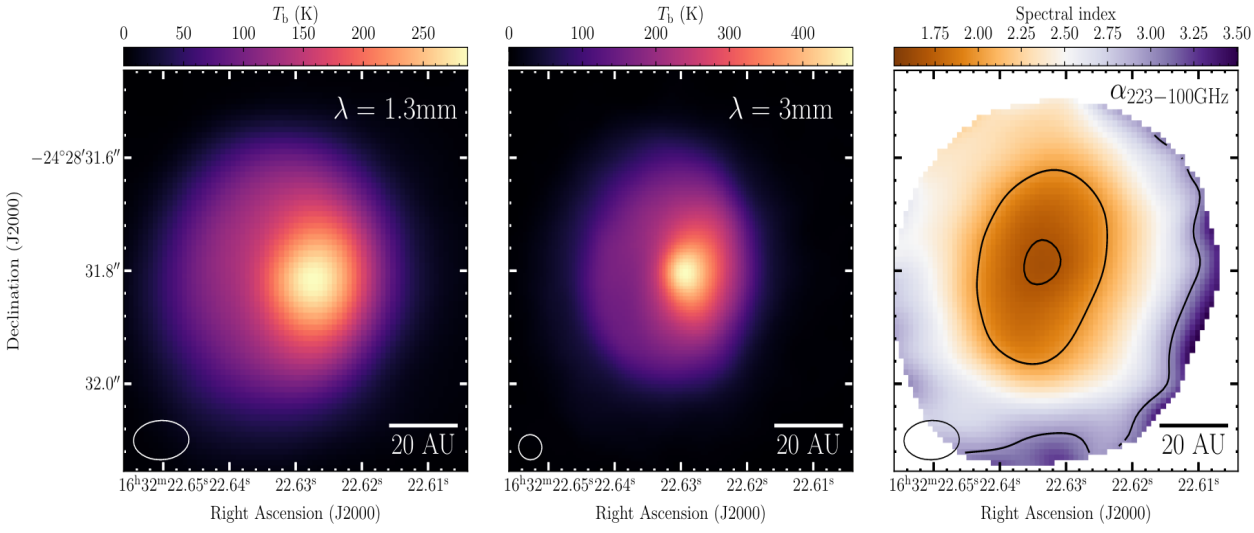

Figure 1: *ALMA observations of IRAS 16293-2422 B in band 6 (left) and 3 (middle) and millimetric spectral index (right).*

Molecular complexity in the cold ISM: Influence of the environment

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Interstellar complex organic molecules (iCOMs), defined as the species containing at least six atoms and the element carbon, are widely found in hot cores and hot corinos. Nowadays, several works reported the detections of iCOMs in cold regions (<20K), like cold clouds and prestellar cores. Those detections challenge the early models which predicted that simple species were produced during the cold phases of the star formation process and frozen into the grain mantles, enabling the formation of more complex species, like the iCOMs, in the grain surfaces at lukewarm temperatures. To better constrain the process of iCOMs formation during the early evolutionary stages of star formation, we conducted pointed observations toward three prestellar core candidates in different environments (high latitude cloud, Strömgren sphere, filamentary cloud) using the IRAM-30m telescope in the frequency range from 79 to 102 GHz. The prestellar core candidates were selected from the Herschel Galactic Cold Core Catalog (GCC). In this work, we present the results of line identification, column densities, molecular hydrogen density and kinetic temperature derived by LTE/non-LTE computations. We detected up to 35 species and 68 transitions in these cores with variations in terms of molecular complexity. Deuterium species which are typical tracers of prestellar cores are detected in two cores, suggesting that the core without deuterium species is less evolved. Based on the ionic species and Nahoon chemical modelling, we estimate the cosmic ray ionization rate in each core, which is an important environmental parameter for iCOM formation and desorption. We will present the molecular complexity in these three cores which will be later better constrained with VLA and GBT NH_3 observations as well as mapping observations of molecular ions.

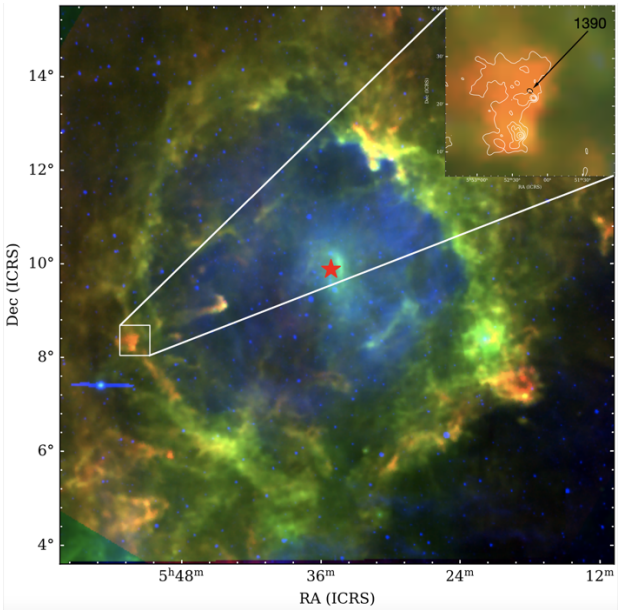

Figure 1: *The rgb figure of λ Orionis, the host region of one of our cores 1390. The upper right corner zooms in on the 1390 core. Blue: Ha emission (VTSS); green: 100 μm emission (IRAS); red: 353 GHz emission (Planck). The zoomed figure is overlaid by contours of the Herschel 250 μm emission with the levels of [3, 5, 7, 10, 20] ×σ. The core 1390 is shown by black ellipse*

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POSTER CONTRIBUTIONS

Microwave and Millimeter Laboratory Spectroscopy of Allylimine

D. Alberton[1], L. Bizzocchi[2,3], M. Melosso[3], N. Jiang[3], V. M. Rivilla[4,5], A. Pietropolli Charmet[6], P. Caselli[1]

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The interstellar medium (ISM) is filled with complex organic molecules (COMs), some of which are building blocks of pre-biotic species. COMs are also important to trace the physical properties of star and planet-forming regions. It is therefore important to understand the ISM chemical inventory and shed light on the COMs formation routes. Of particular interest are the precursors of ammino acids, the building blocks of proteins. So far, ammino acids have been found in large amount in primitive meteoritic material in the Solar System, such as carbonaceous chondrites, while only Glycine has been found in the comet 67P/Churyumov-Garasimenko. In the ISM, only a few ammino acid precursors have been detected and more work is needed to unveil the interstellar paths to these pre-biotic molecules. In this work we focus on an important missing piece, Allylimine (CH_2=CH-CH=NH), shown in Figure 1. We present here the microwave and millimeter spectroscopic characterization of Allylimine. The analysis, supported by high-level quantum chemical ab initio calculations, has been carried out employing the Center for Astrochemical Studies Absorption Cell (CASAC) at the Max-Planck-Institute für extraterrestrische Physics and the University of Bologna frequency modulation spectrometers. The measurements, up to 310 GHz, allowed the ground rotational state characterisation of Allylimine and provided the parameters to create the most reliable catalog to date for its detection in the ISM.

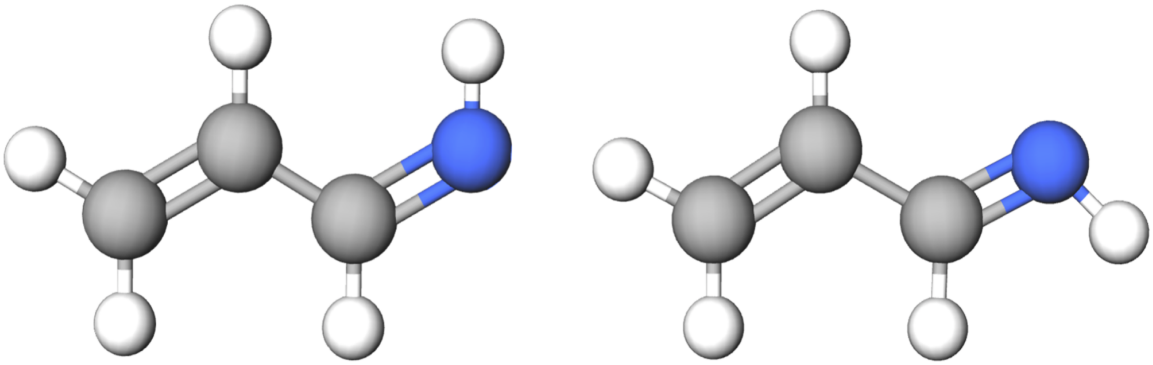

Figure 1: *Allylimine rotamers. From left to right, TS and TA.*

High Level *ab initio* Binding Energy Distribution of Molecules on Interstellar Ices

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The binding energy is a parameter of central importance for astrochemical models. We proposed[1] a new procedure to compute binding energy distributions of atoms and molecules on interstellar ice model surfaces, based on *ab initio* molecular dynamics and density functional theory (DFT), validated by high-level *ab initio* methods at a CCSD(T)/CBS level.

The pipeline consists of three steps: (1) Extensive DFT benchmark on small water clusters (2) Modeling of amorphous solid water (ASW) surfaces using *ab initio* molecular dynamics. (3) Sampling of the binding sites on the surface with the target molecule and computation of the binding energies.

We have applied the procedure to hydrogen fluoride (HF), a promising tracer of the molecular content of galaxies, using a 22-water molecules surface. We found 255 unique structures corresponding to 3 different binding modes and a binding energy distribution (**Figure 1**) with an average value of 5313 ± 74 K, and a dispersion of 921 ± 115 K.

I will present the advantages of this pipeline and how it can be employed to build an accurate and reliable binding energy distribution database of molecules on ASW and other astrophysically relevant surfaces.

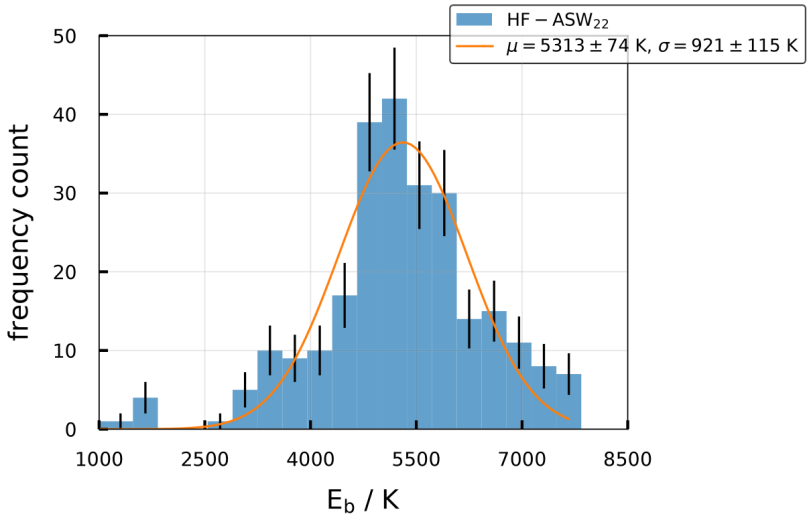

Figure 1: *Histogram of the binding energy distribution obtained for the HF–ASW system.*

1. G. Bovolenta, S. Bovino, E. Vöhringer-Martinez, D. A. Saez, T. Grassi, S. Vogt-Geisse, *Molecular Astrophysics*, **2020**, 21, 100095

2. T. Grassi, S. Bovino, P. Caselli, G. Bovolenta, S. Vogt-Geisse, B. Ercolano, *A&A* **2020,** 643, A155

Study of Fischer-Tropsch-type reactions in chondritic meteorites

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The outcome of organic chemical reactions in the dust grains present in protostellar envelopes and protoplanetary disks are of significant importance, since evidence demonstrates that reactions can be promoted with the interaction of the reactants with the solid phase, or the ices that covers them[1,2,3]. With time, primordial grains coagulated and were processed to form bigger objects in the Solar System. During the late periods of Earth formation, the infall of these materials into the planet's surface could have brought an important amount of organic matter, as well as contributed to its chemical enrichment by promoting organic synthesis processes.

We will present laboratory experiments where we attempted the synthesis of simple organic molecules, such as hydrocarbons and alcohols, via FT-type reactions supported by different chondritic materials (ordinary and carbonaceous chondrites) under early-Earth conditions (H_2:CO = 4, ~1 atm and T=200-600 deg). The gas mixtures were introduced in a stainless-steel reactor containing the meteorite samples and the products of the reactions were analyzed in situ by gas chromatography. We report the production of all the products expected from FT reactions, including oxygenated compounds, and discuss the selectivity for the different meteorite samples.

1. R. F. Ferrante, M. H. Moore, J. A. Nuth and T. Smith, *Icarus*, **2000**, 145, 297
2. M. Kress, A. G. G. M. Tielens, *Meteorit. Planet. Sci.,* **2001**, 36, 75-91.
3. H. Linnartz, S. Ioppolo and G. Feedosev, *Int. Rev. Phys. Chem.* **2015**, 34, 205

The Role of Ions in Irradiated Astrophysical Ices

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Cosmic ices contain ions produced by irradiation from cosmic rays and UV photons, yet solid-phase ion-ice reactions are currently ignored in all astrochemical models, even though gas-phase ion-molecule reactions are arguably the single-most important class of reactions in astrochemistry. Thus, developing a model that includes solid-phase ion-ice reactions is essential to accurately model interstellar ice chemistry, especially given the imminent launch of the James Webb Space Telescope.

To fill this gap, we have compiled a solid-phase chemical network for use in a rate-based astrochemical model proposed by Mullikin et. al.[1] which, for the first time, includes ionic species produced via the photoionization of the ice. Using this network, we simulated the photo-irradiation of a pure O_2 ice and plan to constrain photolysis rates through direct comparison with experimental data.

Our preliminary results indicate that, as in the gas, solid-phase ion-ice reactions are very efficient and, indeed, become the dominant formation routes for many species.

1. E. Mullikin, H. Anderson, N. O'Hern, M. Farrah, C. R. Arumainayagam, E. F.van Dishoeck, P. A. Gerakines, A. I. Vasyunin, L. Majumdar, P. Caselli, and C. N.Shingledecker, "A New Method for Simulating Photoprocesses in Astrochemical Models," *The Astrophysical Journal*, vol. 910, p. 72, Mar. 2021.

Unveiling Interstellar Complex Organic Molecules in the highly obscured Class 0 protostar NGC 1333 IRAS 4A1

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Since the discovery, almost 20 years ago, of interstellar complex organic molecules (iCOMs) toward Sun-like protostars, less than twenty of hot corinos are currently known. Hot corinos are compact (< 100 au), hot (T> 100 K) and dense ($n(H_2)>10^7$ cm^{-3}) regions in the close vicinity of low-mass protostars displaying a very rich chemistry, specially in iCOMs. The presence of iCOMs in the earliest stages of star formation may have important consequences for the emergence of life, however their formation (gas phase chemistry or dust grain surface chemistry) is still debated. One of the most extensively studied star-forming regions is NGC 1333 in the Perseus molecular cloud, which hosts a Class 0 protobinary system separated by 1.8" (~540 au). The two protostars, named 4A1 and 4A2, display distinct characteristics: while 4A1 is the brightest in dust continuum emission only 4A2 presents a rich hot corino spectrum detected in several iCOMs lines[1,2]. Recently, centimeter observations reveal methanol emission toward both protostars[3]. In this talk, we report the detection of several iCOMS lines in emission toward the highly obscured protostar 4A1 within the framework of the NOEMA Large Program SOLIS. I will present the inventory of iCOMs and the derived abundances in 4A1 and the comparison with its companion 4A2 as well as with the well studied IRAS 16293-2422 binary system. The SOLIS-NOEMA observations allows to attack also in the millimeter regime the study of the chemical composition around 4A1.

1. A. López-Sepulcre, N. Sakai, R. Neri et al. *A&A,* **2017**, 606, A121
2. V. Taquet, A. López-Sepulcre, C. Ceccarelli et al. *ApJ,* **2015**, 804, 81
3. M. De Simone, C. Ceccarelli, C. Codella et al. *ApJ,* **2020**, 896, L3

Quantum chemistry techniques and reactivity in the gas-phase: Theoretical reaction kinetics

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The essential feature of the theoretical reaction kinetics is that the activated complexes are considered to be formed in a state in which they are in equilibrium with the reactants. The reaction rate is the concentration multiplied by the frequency that leads to the products, which is known from kinetic theory. The 3D-space is a very different environment from a typical chemical laboratory. Not only are the resources extremely limited in terms of material, but also temperature and pressure tend to be extremely low. This means that reactions typically considered feasible can become impossible in an astrochemical model, even if the energy requirements are modest. Typically, the energy to proceed is supplied by an initial exothermic addition step.

In this work we present the assumption of the Capture model, shown in the Figure, that any collision (bimolecular) which gets past the centrifugal barrier leads to a successful association. After that, we adopt the RRKM treatment assuming that the states of the reactant side of the barrier are in equilibrium and allow us to use the transition state theory.[1]

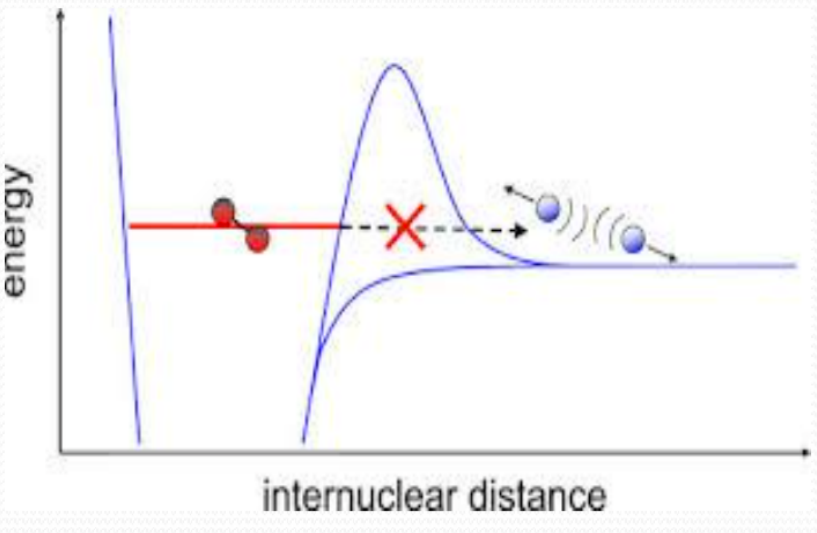

Figure: *The capture model*

1. D. Skouteris, N. Balucani, C. Ceccarelli, N. Faginas-Lago, S. Falcinelli, M. Rosi, MNRAS **2019,** 482 3567–3575

A combined experimental and theoretical investigation of reaction OH+C_2H_4: a possible route to acetaldehyde and vinyl alcohol

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The reaction OH+C_2H_4 has been suggested as a possible formation route of acetaldehyde in the interstellar medium. However, the reaction has an entrance barrier and the room temperature rate coefficient is not large and is supposed to be negligible at low temperatures. However, recent investigations of other OH reactions with organic molecules by the CRESU technique have revealed an unexpected increase of the rate coefficients at very low temperatures (Heard, 2019).

Even though other routes have been recently assessed by Vazart et al. (2020), we have decided to investigate the OH+C_2H_4 reaction with the specific aim to verify whether acetaldehyde is (or not) the main reaction product. In particular, we have used the crossed molecular beam technique with mass spectrometric detection to establish the yield of primary products and we have performed dedicated electronic structure calculations of the potential energy surface with statistical estimates of the product branching ratios. The combined experimental and theoretical study has revealed that H_2CO+CH_3 is by far the dominant channel. Some vinyl alcohol is also formed in a H-displacement mechanism, while the yield of acetaldehyde is really negligible. Data from the SOLIS-NOEMA campaign have been analysed to derive the abundance of acetaldehyde in several low-mass star forming regions resembling the solar nebula from which our Solar System originated.

The main conclusion of this work is that reaction OH+ C_2H_4 cannot be considered one of the main routes of acetaldehyde formation in the conditions of the interstellar medium, but it can be considered a route towards the formation of vinyl alcohol in relatively high energy regions.

1. D. E. Heard, *Acc. Chem. Res.* **2018**, 51, 11, 2620–2627

2. F. Vazart, C. Ceccarelli, N. Balucani, E. Bianchi, D. Skouteris, *MNRAS* **2020**, 499, 4, 5547–5561

UCLCHEMCMC: An MCMC for Inferring Physical Parameter from Emission Lines

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We present a soon to be, publicly available, open source, Markov Chain Monte Carlo inference code, UCLCHEMCMC. This code is designed to estimate physical parameters of an observed cloud of gas, when given the observed values of different emission lines. UCLCHEMCMC runs an inference using a Markov Chain Monte Carlo algorithm, with a Bayesian probability function and a full forward modelling approach, in order to estimate a posterior probability distribution of the physical parameter space. The chemical models and radiative transfer code results created when running UCLCHEMCMC are stored in an SQL database in order prevent redundant model calculations which in turn speeds up the inference the more it is used.

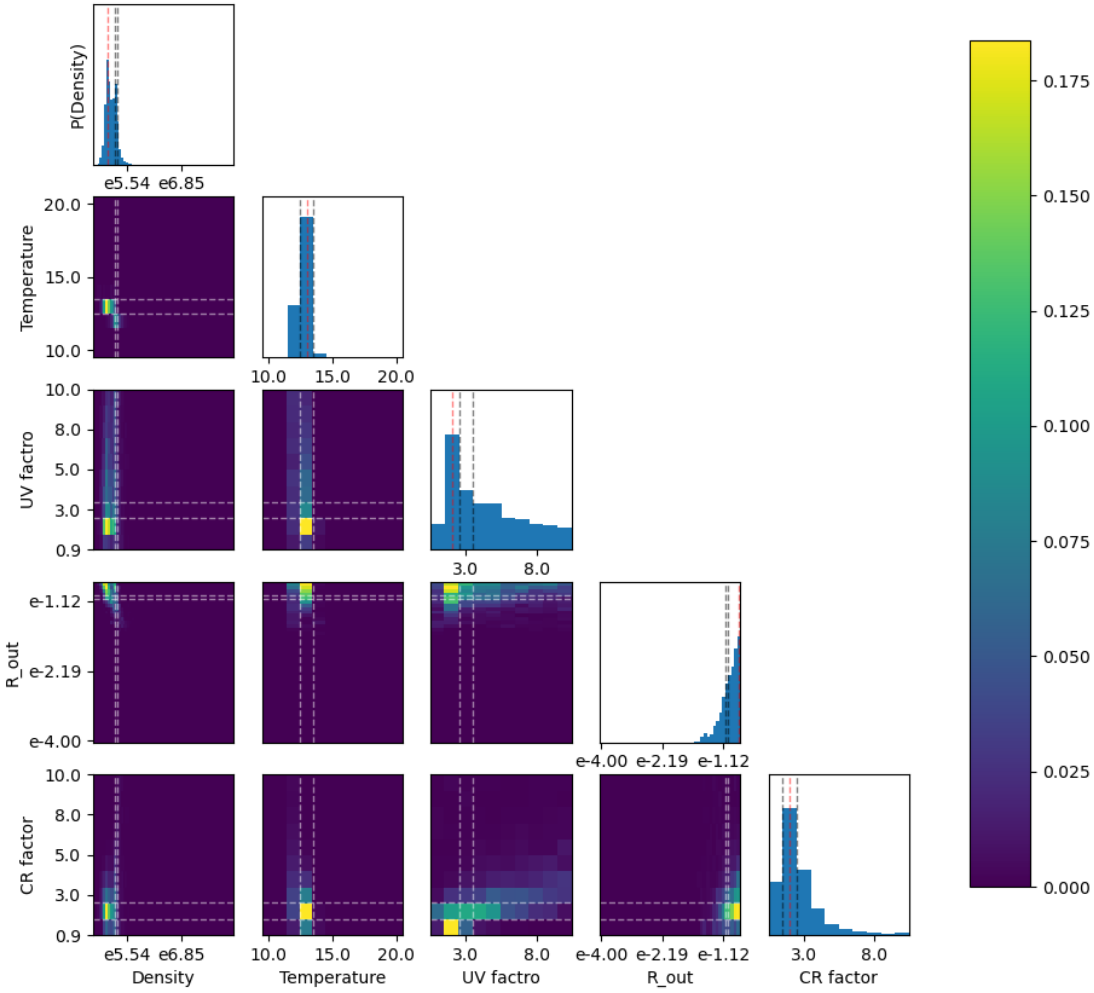

***Figure 1**: Posteriors of Inference on mock data. Black dashed lines indicate the true values*

VUV Photolysis of CO/H_2O Interstellar Ice Analogues: EPR Detection of Radical Intermediary Species and Characterization of Carboxylic Acid Products

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More than 60 interstellar complex organic molecules (iCOMS) have been identified in different interstellar environments including star forming regions and cold dense molecular clouds[1]. The formation mechanisms of these iCOMs are not yet established and could take place either in the gas phase or in the solid phase in interstellar ices, as proposed by many experimental and theoretical works[2,3]. In this contribution, we propose a new experimental approach allowing, in the same set of experiments, the solid phase detection of precursors, radical intermediary species as well as final products. This is possible thanks to the concomitant use of infrared and EPR spectroscopies and mass spectrometry. This unique procedure allows us to detect intermediary species such as H, CH_2OH, and HOCO radicals and stable carboxylic acids such as formic acid (HCOOH) and glycolic acid ($HOCH_2COOH$) from the VUV photolysis of CO/H_2O interstellar ice analogues. As a result, we are able to propose a solid phase formation route for formic and glycolic acids in interstellar ices (see figure 1).

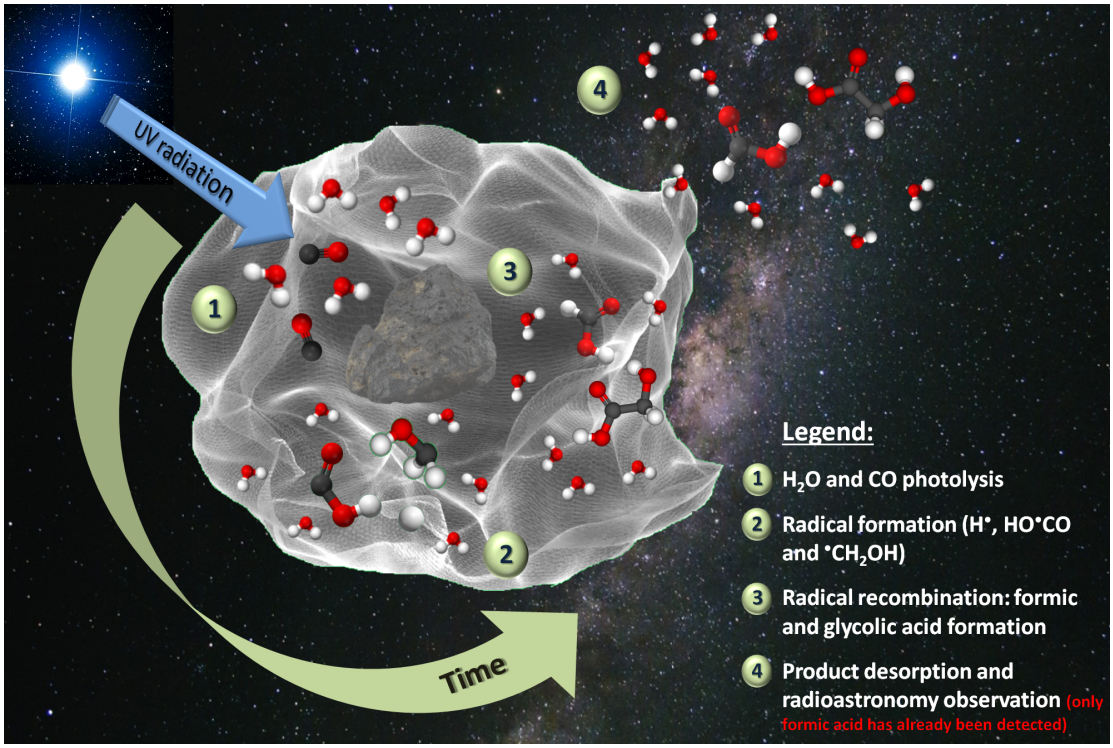

Figure 1: *Proposed solid phase mechanism for formic and glycolic acid in interstellar ices.*

1. B.A. McGuire, *ApJS*. **2018**, 239, 17
2. K.-J. Chuang, G. Fedoseev, D. Qasim, S. Ioppolo, E. van Dishoeck, H. Linnartz, *MNRAS*. **2017**, 467, 2552
3. D. Skouteris, N. Balucani, C. Ceccarelli, F. Vazart, C. Puzzarini, V. Barone, C. Codella, B. Lefloch, *ApJ*. **2018**, 854, 135

A Combined Experimental and Theoretical Investigation of the Reactions $CN(X^2\Sigma^+)$ + HCCCN and $CN(X^2\Sigma^+)$ + H_2CCHCN and Astrophysical Implications

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CN is one of the most abundant and widespread radicals in interstellar space. The fast reactions between CN and unsaturated hydrocarbon molecules generate various nitriles[1,2], including HC_3N and CH_2CHCN, which are known to be prebiotic species. HC_3N is ubiquitous in interstellar environments. Similarly, CH_2CHCN has also been detected in numerous objects, such as dark cloud TMC-1, massive star-forming region in Sgr B2 and Orion KL, circumstellar envelope of the C-rich star IRC +10216, Titan's atmospheres, etc. Because of the wide distribution of these species, it is worthwhile to explore if the reactivity of CN with HC_3N and CH_2CHCN can produce more complex nitriles. Actually, these two reactions have been implemented into the photochemical models of Titan's atmosphere, giving NCCCCN and $C_4H_2N_2$ as the sole product in each reaction. Kinetics studies confirmed that the rate constants for the $CN(X^2\Sigma^+)$ + HC_3N reaction increase rapidly as the temperature decreasing from 300 K to 22 K.[3] However, very few studies have focused on the $CN(X^2\Sigma^+)$ + CH_2CHCN reaction at low temperatures. The rate constants estimated by extrapolating the Arrhenius plot have a huge impact on the precision of astrochemical models. Furthermore, there is no experiment to determine the reaction products. Given these unsolved problems, it is essential to gain further insights into these elementary reactions, either experimentally or theoretically, to verify the accuracy of the developed models or update the existing chemical networks. Obviously, these two reactions are also possible in the interstellar medium (ISM) where CN, HC_3N, and CH_2CHCN are abundant. In our study, we elucidate the reaction mechanism of the $CN(X^2\Sigma^+)$ + HCCCN and $CN(X^2\Sigma^+)$ + CH_2CHCN reactions by combining crossed molecular beam experiments and electronic structure calculations. Rate coefficients will also be estimated at the temperatures of relevance in interstellar clouds. Our preliminary results reveal that in both cases the reactions proceed with the barrierless addition of CN to the unsaturated carbon-carbon bond leading to a bound intermediate, followed by breaking of C-H bond to produce NCCCCN or Z, E-NCCHCHCN product.

Acknowledgements: This research was supported by the Italian Space Agency (ASI, DC-VUM-2017-034, Grant No 2019-3 U.O Life in Space) and the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie project grant agreement No 811312 for the project "Astro-Chemical Origins" (ACO).

1. I. R. Sims, J.-L. Queffelec, D. Travers, *et al.*, *Chem. Phys. Lett*. **1993**, 211, 461-468.
2. N. Balucani, O. Asvany, L. C. L. Huang, *et al.*, *Astrophys. J.* **2000**, 545, 892-906.
3. S. Cheikh Sid Ely, S. B. Morales, J.-C. Guillemin, *et al.*, *J. Phys. Chem. A*. **2013**, 117: 12155-12164.

Glycolaldehyde Formation on Interstel·lar Water Ice Surfaces. A Computational Quantum Chemical Approach

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Observational studies evidence that our universe is filled with chemical diversity[1,2]. Astrochemists of diverse disciplines aim to unfold the intricate chemical mechanisms that occur in space to get insight on one of the primordial questions we have today: what is the origin of life? To evolve from dead chemical matter into living beings, there are some essential chemical compounds that must be present for that to occur, such as amino acids[3] and complex sugars[4,5]. Focusing on sugars, glucose is one of the main targets. However, its presence has not been confirmed in space while this is indeed the case of its closest relative, glycolaldehyde (GLA, HO H_2CHCO)[6]. Nonetheless, chemical reactions and mechanisms through which it can be formed in space are still doubtful[5]. In this contribution, we present results dedicated to GLA formation on surfaces of interstellar water ice adopting the formose reaction, $2 \cdot H_2CO \rightarrow$ GLA, and its radical derivation $H_2CO + HCO^* + H^* \rightarrow$ GLA. Reactions in the gas phase (i.e., absence of water ice) have been used for a benchmarking study, in which CCSD(T) results were compared with those obtained at the more approximated DFT theory level. With the latter, calculations of the GLA formation reactions have been carried out on cluster models for water ice (see Figure 1), in which the energy features of the reactions (i.e., reaction energy and activation energies) are provided. Additionally, simulations also help us to understand the role of the ice surface in this synthetic route.

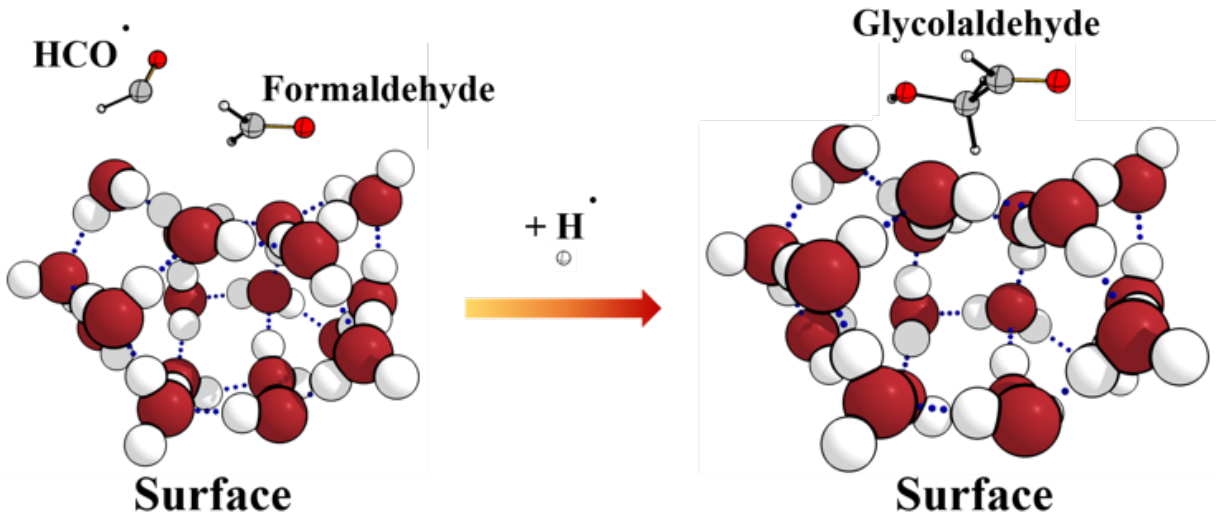

Figure 1: *Glycolaldehyde formation by reaction of HCO with H_2CO followed by H addition simulated on a cluster model mimicking the surfaces of interstellar of water ice.*

1. McGuire, B. A. **2018** *ApJS 239*,17.
2. Botta, O.; Bada, J.L. **2002** *Surv. Geophy.*, *23*, 411-467.
3. Ehrenfreund, P.; Charnley, S. B. **2000** *Annu. Rev. Astron. Astrophys. 38*, 427-83
4. Woods, P.M.; Slater, B.; Raza, Z.; Viti, S.; Brown, W.A.; Burke, D.J. **2013** *ApJ*, *777*, 90.
5. Zellner, N.E.B.; P. McCaffrey, V.; Butler, J.H.E. **2020** *Astrobiology*, *20*, 1377-1388.
6. Jørgensen J.K.; Favre, C.; Bisschop, S.E.; Bourke, T.L.; Dishoek, E.F.; Schmalz, M. **2012** *ApJL 757* L4

Computational Investigation on the Potential Energy Surface Of $H_2CO + NH_2$ → $NH_2CHO + H$ on Interstellar Water Ice Surfaces.

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Formamide is a molecule of interstellar paramount importance because it belongs to the group of the paradigmatic interstellar complex organic molecules (iCOMs)[1]. Moreover, it is also a molecule of particular relevance in prebiotic chemistry as it is the simplest molecule containing the four most essential atoms constituting biological systems (hydrogen, carbon, nitrogen and oxygen), and it is the simplest molecule containing the amide bond O-C-NH, the group that joins amino acids forming peptides[2,3]. Due to its importance, different pathways leading to its interstellar formation has been studied considering both in the gas-phase and on ices of dust grains since it was first detected[2–4]. In the present work, computational simulations based on quantum chemical calculations are presented, focusing on the energetics of its formation from reaction of NH_2 with H_2CO, a channel proposed to occur in the gas phase[3], on water ice surfaces. Simulations are based both cluster and periodic calculations to mimic the water ice surfaces and different DFT functionals have been employed to obtain the potential energy surface of the reaction. Results indicate that the water ice surface favors thermodynamically the reaction, which moreover can be further favored when the final step (i.e., the dehydrogenation of the NH_2CH_2O intermediate) takes place by reaction with an incoming H atom forming H_2.

1. Ceccarelli, C.; Caselli, P.; Fontani, F.; Neri, R.; López-Sepulcre, A.; Codella, C.; Feng, S.; Jiménez-Serra, I.; Lefloch, B.; Pineda, J. E.; Vastel, C.; Alves, F.; Bachiller, R.; Balucani, N.; Bianchi, E.; Bizzocchi, L.; Bottinelli, S.; Caux, E.; Chacón-Tanarro, A.; Choudhury, R.; Coutens, A.; Dulieu, F.; Favre, C.; Hily-Blant, P.; Holdship, J.; Kahane, C.; Al-Edhari, A. J.; Laas, J.; Ospina, J.; Oya, Y.; Podio, L.; Pon, A.; Punanova, A.; Quenard, D.; Rimola, A.; Sakai, N.; Sims, I. R.; Spezzano, S.; Taquet, V.; Testi, L.; Theulé, P.; Ugliengo, P.; Vasyunin, A. I.; Viti, S.; Wiesenfeld, L.; Yamamoto, S. Seeds Of Life In Space (SOLIS): The Organic Composition Diversity at 300-1000 Au Scale in Solar-Type Star-Forming Regions *. *Astrophys. J.* **2017**, *850*, 176.
2. Rimola, A.; Skouteris, D.; Balucani, N.; Ceccarelli, C.; Enrique-Romero, J.; Taquet, V.; Ugliengo, P. Can Formamide Be Formed on Interstellar Ice? An Atomistic Perspective. *ACS Earth Sp. Chem.* **2018**, *2* (7), 720–734.
3. Barone, V.; Latouche, C.; Skouteris, D.; Vazart, F.; Balucani, N.; Ceccarelli, C.; Lefloch, B. Gas-Phase Formation of the Prebiotic Molecule Formamide: Insights from New Quantum Computations. *Mon. Not. R. Astron. Soc. Lett.* **2015**, *453* (1), L31–L35.
4. Enrique-Romero, J.; Rimola, A.; Ceccarelli, C.; Ugliengo, P.; Balucani, N.; Skouteris, D. Reactivity of HCO with CH3 and NH2 on Water Ice Surfaces. A Comprehensive Accurate Quantum Chemistry Study. *ACS Earth Sp. Chem.* **2019**, *3* (10), 2158–2170.

Modernised Cosmic Ray Chemistry – UCLCHEM

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Cosmic rays play a vital role in the chemistry of cold (10-30K), dense (>10^2cm^{-3}) molecular clouds. While they can pierce deep into these regions, they are also attenuated by collisions as they travel. This leads to the cosmic ray ionisation rate and the cosmic ray H_2 dissociation rate to be dependent on the density of the system. Previously, using Voyager data, polynomial fits for the upper and lower limits of these dependencies were created[1,2]. These dependencies, alongside the production and reaction of excited species[3], have been included into a gas-grain chemical code, UCLCHEM. These additions have been applied to the cases of prestellar cores to determine the chemical significance during this crucial stage while making comparisons to observations of cores like L1544.

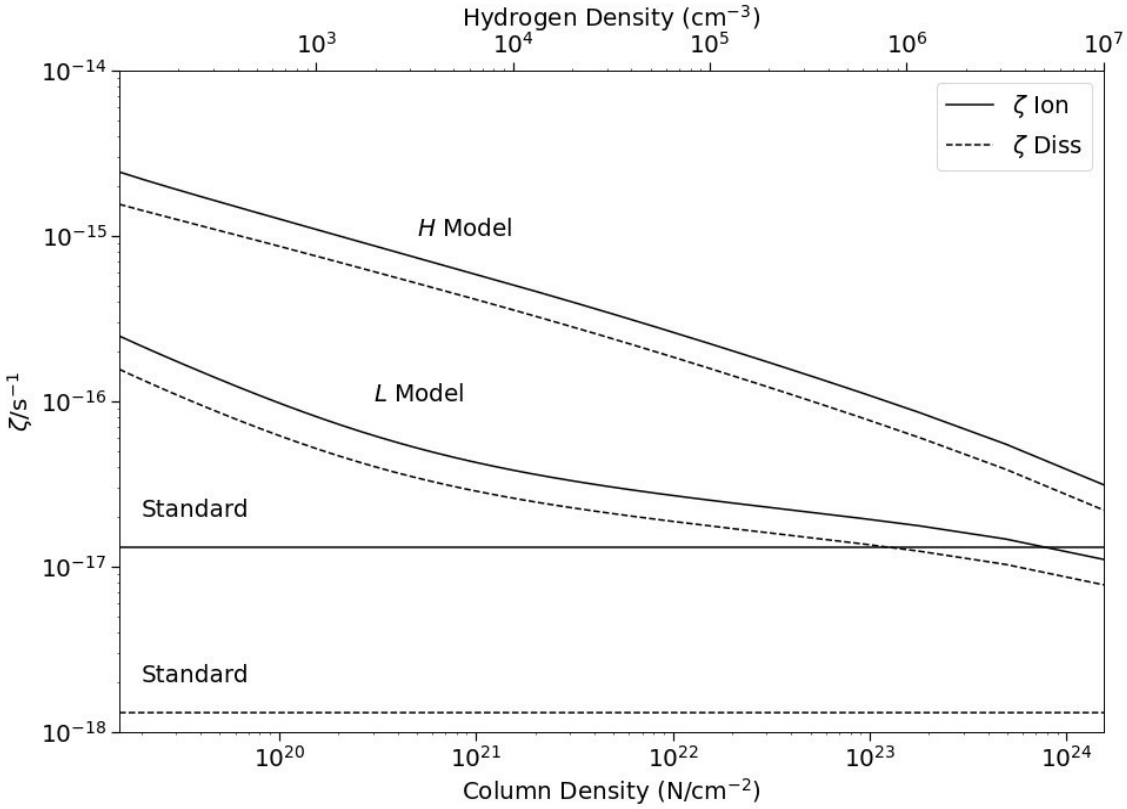

Figure 1: *Figure showing the ionisation rate and H_2 dissociation rate dependencies compared to UCLCHEM's standard handling.*

1. M. Padovani, D. Galli, A. Ivlev, P. Caselli, A. Ferrara, A&A 619 A144 (2018), DOI: 10.1051/0004-6361/201834008

2. M. Padovani, A. Ivlev, D. Galli, P. Caselli, A&A 614 A111 (2018), DOI: 10.1051/0004-6361/201732202

3. C. N. Shingledecker, J. Tennis, R. Le Gal, E. Herbst, (2018), The Astrophysical Journal, 861, 20

Quantum Chemical Calculations of Binding Energies of Astrochemically-Relevant Sulphur-Containing Species on Amorphous Water Ice Mantles

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In the interstellar medium (ISM), i.e. the matter filling the space between the stars, it is possible to find different environments, depending on density, temperature, and chemical composition. Among them, we find molecular clouds, often referred to as the cradle of stellar birth.[1] Indeed, there, radio to far-infrared observations revealed the presence of several molecules in the gas phase, while near-infrared spectroscopy detected the existence of submicron sized dust grains covered by H_2O-dominated ice mantles, which are often called "dirty ices" due to the presence of other volatile species.[2] The interaction between gas-phase species and the surfaces of water ices is measured by the binding energy (BE), a crucial parameter in the astrochemical numerical models that describe the evolution of the ISM chemistry. The aim of this work is to provide the BEs of a set of sulphur-containing species. To this purpose, adsorption of the species on two water ice mantles, the former modelled by the (010) surface of a proton-ordered crystalline ice model and the latter consisting in an amorphous water ice model, has been performed. The Density Functional Theory (DFT)-based B3LYP-D3(BJ) and M06-2X functionals were used for the prediction of the structures and energetics.[3] The DFT BEs computed with the crystalline ice models were refined by adopting an ONIOM-like procedure to estimate the correction at CCSD(T) level toward complete basis set extrapolation. Results indicate that full DFT BEs are very close to those corrected at CCSD(T) level. Moreover, as the time-limiting step is the geometry optimization of the structures, we developed a cost-effective recipe to arrive at the BE values of the same quality as those computed at full DFT level. We adopted the computationally cheaper HF-3c method to optimize the geometries, while the final BE were obtained by single point energy calculations at DFT on the HF-3c optimized geometries. Comparison between DFT//HF-3c and full DFT BE values showed a very good linear correlation between the two sets of data, validating the proposed procedure, which was subsequently applied to compute the BEs with the amorphous surface model, allowing a wide exploration of different binding sites in an affordable way. Computed data were compared with the available literature data.[4,5]

1. P. Caselli, C. Ceccarelli, *Astron. Astrophys. Rev.* **2012**, 20, 56
2. A.A. Boogert, P.A. Gerakines, D.C. Whittet, *Annu. Rev. Astron. Astr.* **2015**, 53, 541-581
3. S. Ferrero, L. Zamirri, C. Ceccarelli, A. Witzel, A. Rimola, P. Ugliengo, *ApJ*, **2020**, 904, 11-30
4. A. Das, M. Sil, P. Gorai, S.K. Chakrabarti, J.C. Loison, *ApJS*, **2018**, 237, 9-21
5. V. Wakelam, J.C. Loison, R. Mereau, M. Ruaud, Molecular Astrophysics, *Mol.Astrophys.* **2017**, 6, 22-35

Structures and Properties of Known and Postulated Interstellar Cations

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Positive ions play a fundamental role in the interstellar chemistry[1,2], especially in cold environments where chemistry is believed to be mainly ion-driven. However, in contrast with neutral species, most of the cations present in the astrochemical reaction networks are not fully characterized in the astrochemical literature. To fill up this gap, we have carried out new accurate quantum chemical calculations to identify the structures and energies of 262 cations with up to 14 atoms that are postulated to have a role in the interstellar chemistry. Optimised structures and rotational constants were obtained at M06-2X/cc-pVTZ level, while electric dipoles and total electronic energies were computed with CCSD(T)/aug-cc-pVTZ//M06-2X/cc-pVTZ single point energy calculations. The present work complements the study by Woon & Herbst (2009)[3], who characterised the structure and energies of 200 neutral species involved as well in the interstellar chemistry. Taken together, the two datasets can be used to estimate whether a reaction, postulated in present astrochemical reaction networks, is feasible from a thermochemistry point of view and, consequently, to improve the reliability of the present networks used to simulate the interstellar chemistry. We provide an actual example of the potential use of the cations plus neutral datasets. It shows that two reactions, involving Si-bearing ions and present in the widely used reaction networks KIDA and UMIST, cannot occur in cold ISM because endothermic.

1. W. D. Watson, *The Astrophys. J.* **1973**, 183, L17
2. E. Herbst, W. Klemperer, *The Astrophys. J.* **1973**, 185, 505-534
3. D. E. Woon, E. Herbst, *The Astrophys. J. Sup. Series* **2009**, 185, 273

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