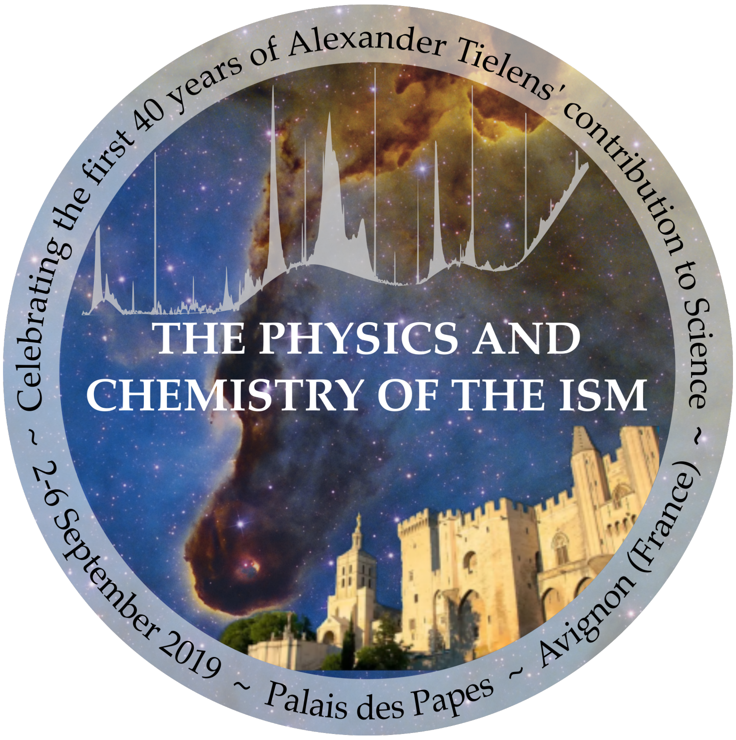
THE PHYSICS AND CHEMISTRY OF THE INTERSTELLAR MEDIUM

Celebrating the first 40 years of Alexander Tielens' contribution to Science



Book of Abstracts

Palais des Papes - Avignon - France
2-6 September 2019

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UGA Univ. Grenoble Alpes
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IPAG Institut de Planétologie et d'Astrophysique de Grenoble
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SRON Netherlands Institute for Space Research
NWO Netherlands Organisation for Scientific Research
euro-PAH


~ Celebrating the first 40 years of Alexander Tielens' contribution to Science ~
2-6 September 2019 ~ Palais des Papes ~ Avignon (France)

CONFERENCE PROGRAM

Monday 2 September 2019

Time		**Speaker**
10:00	Registration	
13:00	Registration & Welcome Coffee	
13:30	Welcome Speech	C. Ceccarelli
	Opening Talks	
13:40	PhD years	H. Habing
13:55	Xander Tielens and his contributions to understanding the ISM	D. Hollenbach
	The Dust Life Cycle	
14:20	Review: The dust cycle in galaxies: from stardust to planets and back	R. Waters
14:55	The properties of silicates in the interstellar medium	S. Zeegers
15:10	3D map of the dust distribution towards the Orion-Eridanus superbubble with Gaia DR2	S. Kh. Rezaei
15:25	Invited Talk: Understanding interstellar dust from polarization observations	F. Boulanger
15:50	Coffee break	
16:20	Review: The life cycle of dust in galaxies	M. Meixner
16:55	Dust grain size distribution across the disc of spiral galaxies	M. Relano
17:10	Investigating interstellar dust in local group galaxies with new UV extinction curves	G. Clayton
17:25	Invited Talk: The PROduction of Dust In GalaxIES (PRODIGIES)	C. Kemper
17:50	Unravelling dust nucleation in astrophysical media using a self-consistent, non steady-state, non-equilibrium polymer nucleation model for AGB stellar winds	L. Decin
19:00	Dining Cocktail	

Tuesday 3 September 2019

08:15	Registration	
	PDRs	
09:00	Review: The atomic to molecular hydrogen transition: a major step in the understanding of PDRs	E. Roueff
09:35	Invited Talk: The Orion Bar: from ALMA images to new dynamic PDR models	J. Goicoechea
10:00	[CII] optical depth and self-absorption in M17SW	C. Guevara
10:15	Coffee break & Posters	
11:15	Review: PDRs near and far: the extraordinary utility of photodissociation region models	M. Kaufman

Time		Speaker
11:50	The importance of the atomic history in time-dependent simulations of the interstellar gas- from non-thermal to thermal distributions	M. de Avillez
12:05	The physical state of CO-dark gas in the Perseus arm	M. Busch
12:20	Lunch break & Posters	
14:30	The low-metallicity ISM of dwarf galaxies: the multiphase structure and the CO-dark gas	S. Madden
14:45	The atomic envelope of molecular clouds as revealed by machine vision	J.D. Soler

PAH

15:00	Spectroscopy of interstellar polyaromatic hydrocarbons and their photoproducts	J. Bouwman
15:15	Unravelling spectral signatures and photochemical processes of polycyclic aromatic hydrocarbons	A. Petrignani
15:30	Coffee break & Posters	
16:25	Tracing PAH size in prominent nearby mid-infrared environments	C. Knight
16:40	Radioastronomical observations of PAHs and other aromatic species at the earliest stages of star formation	B. McGuire
16:55	Formation process of small hydrocarbons in PDRs: gas phase chemistry or fragmentation of polycyclic aromatic hydrocarbons (PAHs)?	M. Tiwari
17:10	Review: Today's PAH model: four not so easy pieces	L. Allamandola

Wednesday 4 September 2019

08:15	Registration	

PAH

09:00	Review: Astro-PAHs: a journey from space to the laboratory	C. Joblin
09:35	PAHs on/in water ice: structures, energetics, and spectra from FTIR experiments and a multi-method theoretical study	J. Mascetti
09:50	Photoionization of polycyclic aromatic hydrocarbons: contribution to the heating of the Interstellar Medium	P. Bréchignac
10:05	Invited talk: ISM spectra from near- to mid-infrared	T. Onaka
10:30	Coffee break & Posters	
11:35	Experimental studies of the catalytic role of oxygen functionalized PAHs	R. Jaganathan

Ices

11:50	Review: From simple to complex molecules in interstellar ices	A. Boogert
12:25	Ices in small dense molecular cores	L. Chu
12:40	Formation of molecules on cold interstellar grains	F. Dulieu
12:55	Lunch break & Free afternoon	

Thursday 5 September 2019

Time		Speaker
08:15	Registration	
	Ices	
09:00	Review: From astrochemistry to astrobiology? A few selected papers on cosmic ices evolution	L. d'Hendecourt
09:35	SPHEREx: surveying the milky way in biogenic ices	G. Melnick
09:50	Adsorption of volatile molecules on interstellar carbonaceaous analogs	B. Mate
10:05	Invited talk: Laboratory investigations on the chemical and optical properties of interstellar ice analogs	M.E. Palumbo
10:30	Coffee break & Posters	
11:30	Quantum chemistry computations as an interpretative and predictive tool for grain-induced astrochemical processes. The formamide formation case	A. Rimola
11:45	The physics and chemistry on the surface of cosmic dust grains	A. Potapov
12:00	H_2 and HCO^+ formation at the interface with crystalline models of icy mantles: insights from periodic DFT-MD simulations	S. Pantaleone
12:15	Damaged water ice: an opportunity for reactivity?	A. Markovits
12:30	Lunch break & Posters	
	Astrochemistry	
14:30	Review: Carbon chemistry in evolved stars	J. Cernicharo
15:05	Invited talk: Molecular complexity in solar-type star forming regions	B. Lefloch
15:30	IRAM hunt for hot corino and WCCC objects in the OMC-2/3 filament	M. Bouvier
15:45	First astrophysical detection of the helium hydride ion HeH^+	R. Guesten
16:00	Coffee break & Posters	
17:00	Astrochemistry of protoplanetary disks from an observational point of view	C. Favre
17:15	Modelling of the chemistry of protoplanetary disks	M. Ruaud
17:30	Chemistry and isotopic ratios in intermediate redhisft molecular absorbers	S. Wallstrom
17:45	The effect of circumstellar dust grains on the gas phase chemistry in AGB outflows	M. Van De Sande
20:00	Social dinner	
21:30	After dinner speaker	M. Wolfire

Friday 6 September 2019

Time		Speaker
08:15	Registration	
	Astrochemistry	
09:00	Review: Gas-phase chemistry in the interstellar medium: there is still much to learn	N. Balucani
09:35	Prevalent complex organic molecules towards prestellar cores in the Taurus star forming region	S. Scibelli
09:50	Invited talk: Grain surface chemistry and its impact on the gas phase	S. Cazaux
10:15	A computational study of the reaction N(2D)+C_6H_6: implications for the upper atmosphere of Titan	D. Skouteris
10:30	Coffee break & Posters	
	Future & Perspectives	
11:00	Review: Future developments of IRAM instruments	K. Schuster
11:25	Review: Observing facilities for astrochemistry: evolution and future perspectives	T. de Graauw
11:50	Review: Astrochemistry: the next 40 years	E. van Dishoeck
12:15	Closing talk	T. Millar

ORAL CONTRIBUTIONS

Today's PAH model: four not so easy pieces

Louis Allamandola[1*†]

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Over the past thirty-five years the interstellar PAH hypothesis has been tested, has had predictions borne out, and has been successfully applied to a surprising number of disparate astrophysical and astrochemical processes. Along the way, the PAH hypothesis became the PAH model. This progress has only been possible thanks to the close collaboration between laboratory experimentalists, astronomers, modelers and theoreticians. Due to the deep interdisciplinarity of the "PAH Problem" however, this progress has been made in 'fits and starts', and often in choppy, unconnected steps with the result that today's model is not yet as fully integrated into a whole as it can be. Adding to the complexity, since astronomical PAHs are nano-sized molecules, not particles, they play astrophysical and astrochemical roles that differ from those of grains. Given the information PAH spectra contain about the astronomical objects in which they are found, and the key roles they are now called upon to play in the astrophysics of many (if not most) objects across the Universe, sharpening the model as much as it can be sharpened is key to its full exploitation as a novel and far-reaching astronomical tool. This is particularly critical now with the anticipated launch of the *James Webb Space Telescope* (*JWST*) in about two years. *JWST*'s combination of unprecedented sensitivity, spectral resolution, and wavelength coverage will make it possible, for the first time, to measure and fully characterize PAH spectra across the complete 1 - 28 μm range, the range in which the strongest PAH fundamental bands and associated features fall.

Interstellar PAH mid-IR emission spectra form the foundation on which the entire PAH model rests. While great progress has been made in understanding the general spectroscopy of such large molecules, very significant challenges regarding important spectroscopic details remain. Similarly with PAH growth and destruction. Until recently the stepwise processes invoked to grow simple molecules containing a few carbon atoms to polycyclic aromatic structures and fullerenes were very general. Now there are a number of experimental and theoretical studies that show generalizations do not capture PAH growth, destruction and evolution well. Likewise with more complex chemistry involving PAHs. The recent, exciting discovery of benzonitrile in the cold core TMC-1 is the tip of an iceberg. Pun intended. Over the past decade or two, sophisticated experimental work has revealed some of the steps involved in the growth and destruction of PAHs in the gas. This depth of understanding does not yet hold for interstellar ice chemistry involving PAHs. It is critically important to gain this knowledge because a number of laboratory studies of interstellar ice analogs and models show that the inclusion of PAHs can profoundly influence ice chemistry and physics. Taken together, these gaps in our detailed knowledge severely limit what astronomical PAHs tell us today versus what they can tell us.

This talk will touch on some of the recent laboratory advances and challenges in four areas: PAH spectroscopy, growth, destruction, and chemistry.

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

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After the "scoundrels rule" according to which the formation of hydrides is due to processes occurring on the surface of the icy mantles of interstellar grains [1], it has been 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 temperature for several reactions characterized by a significant energy barrier [4]. In addition, the deuteration of interstellar complex organic molecules can well be explained by gas-phase processes [5], while ice chemistry fails to do so [3].

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.

References:
[1] S. Cazaux, AGGM Tielens, C Ceccarelli et al., ApJ, 2003, 593, L51
[2] RT Garrod, SL Widicus Weaver, E Herbst, 2008, ApJ, 682, 283
[3] JK Jorgensen, HSP Muller, H Calcutt et al., A&A, 2018, 620, A170
[4] A Potapov, A. Canosa, E. Jimenez, B. Rowe, Angew. Chem. Int. Ed., 2017, 56, 8618
[5] D Skouteris, F Vazart, C Ceccarelli et al, MNRAS, 2017, 468, L1

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From simple to complex molecules in interstellar ices

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The molecular complexity as we see it in even the most primitive Solar System bodies may well have its origin in dense clouds and protostellar envelopes. Early models by Tielens & Hagen (A&A 114, 245, 1982) calculated that chemistry on the surfaces of cold dust grains in dense clouds forms icy mantles rich in simple molecules, as a result of favorable accretion, diffusion, reaction, and desorption rates. In the subsequent four decades, infrared spectroscopy of dense clouds and protostars have provided observational constraints (e.g., Boogert et al., ARAA 53, 541, 2015), and laboratory experiments have tested and quantified the reaction schemes (e.g., Linnartz et al., IR Phys. Chem. 34, 205, 2015). The interplay between models, experiments, and observations has indeed been impressive, but at present many questions still surround the formation of complex, and even simple, molecules. Much of this is due to a lack of observational constraints. Why does the abundance of CH_3OH ice, an important precursor to complex molecules, vary so much in different clouds, even at comparable cloud depths? Prominent absorption features are still not securely identified. The abundance of simple species, e.g., H_2S, SO_2, H_2CO, HDO, is uncertain. Maps of H_2O, CO, CO_2, and CH_3OH ice abundances in dense clouds and protostellar envelopes would enable better links with gas measurements (IRAM, ALMA), as well as the physical conditions, processes (energetic processing), and time scales, but are still very rare in 2019. Species more complex than CH_3OH were tentatively detected in just a few sight-lines. Several of these issues are fundamentally limited by vibrational spectroscopy (low sensitivity, mode confusion), but at present the lack of suitable instruments and telescopes is to blame. I will summarize recent ice observations, discuss what can be expected from the future missions JWST and SPHEREx (see also talk by G. Melnick), and what we learned from the comparison with in situ measurements of cometary salts, and volatiles, e.g., sulfur-bearing molecules.

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Understanding interstellar dust from polarization observations

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For a long time, polarization has been a secluded facet of interstellar dust studies involving a small number of experts. Today, this research field is expanding as a wealth of observations is becoming available. Like IRAS three decades earlier when it opened the far-IR sky to astronomy, Planck triggered this new era providing us with the first all-sky survey of polarized dust emission. Detailed imaging observations of dust polarization carried out by balloon-borne experiments BLASTPOL and PILOT, the far-IR HAWC+ camera on board of SOFIA and imaging at sub-mm/mm wavelengths from large dish telescopes and ALMA, complement the broad view. The new data are bringing up surprises that upset anticipated results and call for a revised understanding of interstellar dust, accounting for the polarization properties of grains. Conversely, understanding dust polarization has become essential to make use of the data to map the structure of interstellar magnetic fields from the diffuse interstellar medium to pre-stellar cores. My presentation will highlight the main results coming out of the observations and how they contribute to our understanding of interstellar dust.

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IRAM hunt for hot corino and WCCC objects in the OMC-2/3 filament

Mathilde Bouvier[1*†], Ana Lopez Sepulcre[2,1], Cecilia Ceccarelli[1], Claudine Kahane[1], Muneaki Imai[3], Nami Sakai[4], Satoshi Yamamoto[3], Paul Dagdigian[5]

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The Solar System was born 4.5 billion years ago from a clump of a molecular cloud of the Milky Way. Very likely, it was surrounded by numerous high- and low- mass forming stars. Central questions of Astronomy are (1) what happened to the first phases of the Solar System formation and (2) how they might have influenced the appearance of life on Earth.

Chemistry is a powerful tool to answer these questions. For example, 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, allowing the chemical enrichment and diversity of the protostar environment [1, 2]. Hot corinos and Warm Carbon Chain Chemistry (WCCC) objects are two extreme chemically distinct types of solar-mass protostars and are key pieces of evidence of this chemical diversity. On the one hand, hot corinos are dense, hot, and compact (less than 100 au) regions, enriched in interstellar Complex Organic Molecules [3]. On the other hand, WCCC protostars have an inner region deficient in iCOMs but a larger zone (a few thousands of au) enriched in hydrocarbons [4]. Our Sun having been formerly a protostar, an obvious question is whether it experienced a hot corino phase, a WCCC phase or neither during its youth. In this context, we carried out a systematic study to determine whether hot corinos or WCCC objects are present in a region similar to the nursery where the Solar System was born and what could cause their occurrence. To this end, we searched for hot corinos and WCCC candidates in the OMC-2/3 filament, the nearest high- and low- mass star formation region, and the best-known analog of our Sun's birth environment [5, 6]. We used the IRAM 30m and NRO 45m telescopes to observe CH_3OH and CCH, two species enhanced in hot corinos and WCCC objects respectively [7], to determine the chemical nature of nine protostars along the OMC-2/3 filament. In order to disentangle the contribution to the line emission from the parent cloud, we also obtained a map. We carried out a non-LTE analysis of the observed line emission towards the targeted sources and the extended map using the recent collision coefficients for CCH-H_2 computed [8]. We found that the gas emitting the CCH and CH_3OH lines is cold (10-15 K) and dense ($\sim 10^6$ cm^{-3}). Remarkably, the temperature and density are rather constant throughout the filament and do not vary with the position of the sources, suggesting an external origin of the molecular emission.

Therefore, our first results show that, with single-dish observations, we cannot disentangle the emission of the protostars envelope from that of the parent cloud, as assumed in previous works [7, 9]. This brings back the number of definitively classified hot corinos versus WCCC objects to less than a dozen, calling for urgent studies with millimeter interferometers, like IRAM/NOEMA and ALMA.

References:

[1] Cazaux et al., ApJ 593, 51, 2003
[2] Jørgensen et al., A&A 595A, 117, 2016
[3] Ceccarelli et al., propel.conf 47C, 2007
[4] Sakai & Yamamoto, ChRv, 113, 8981, 2013
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[6] Pfalzner et al., PhyS, 90f8001P, 2015
[7] Higuchi et al., ApJS, 236, 52, 2018
[8] Dagdigian, MNRAS, 479, 3227 , 2018
[9] Öberg et al., ApJ, 788, 68, 2014

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Spectroscopy of interstellar polyaromatic hydrocarbons and their photoproducts

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The presence of interstellar polycyclic aromatic hydrocarbons (PAHs) is inferred from the mid-infrared (mid-IR) emission bands that are observed at 3.3, 6.2, 7.7, 8.6 and 11.2 mm. This IR radiation is emitted as the PAHs cascade down to the ground state after they have been excited by interstellar (vacuum) ultraviolet radiation. [1] PAHs have been observed towards a large number of galactic and extragalactic sources and it has been derived that PAHs constitute up to 15% of the total cosmic carbon budget, emphasizing their importance in the cosmic cycle of matter.

Energetic processing of interstellar polyaromatics may result in ionization and/or dissociation. It has been hypothesized that this chemical evolution is reflected in changes in the observed mid-IR emission bands. Observational and laboratory data suggest that dissociation of large interstellar polyaromatics eventually results in formation of fullerenes. The underlying processes involved in the dissociation of aromatics are not yet understood.

Our group characterizes the dissociation of polyaromatics by means of laboratory-based measurements as well as measurements at large-scale facilities such as synchrotron and Free Electron Laser facilities. By combining these techniques with quantum chemical computations we obtain insight in PAH spectroscopy [2] and the dissociation of aromatics at a molecular level of detail [3, 4]. I will review some of our recent results and will emphasize their importance in light of astronomical observations.

Acknowledgments:

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References

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[2] J. Bouwman, P. Castellanos, M. Bulak, et al., A.G.G.M. Tielens, *A&A* 2019, 621, A80.
[3] J. Bouwman, A.J. de Haas, J. Oomens, *Chem. Commun.* 2016, 52, 2636-2638.
[4] A.J. de Haas, J. Oomens, J. Bouwman, *Phys. Chem. Chem. Phys.* 2017, 19, 2974-2980.

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Photoionization of polycyclic aromatic hydrocarbons: contribution to the heating of the interstellar medium

Philippe Brechignac[1*], Laurent Verstraete[2†], Emmanuel Dartois[1], Joffrey Fréreux[1], Ozan Lacinbala[1], Laurent Nahon[3], Helgi Hrodmarsson[3], Gustavo A. Garcia[3]

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Polycyclic aromatic hydrocarbons (PAHs) are chemical species encountered in a very large variety of environments, in particular in combustion media. They are potential carriers to explain the infrared emission mechanism at the origin of the "unidentified infrared" (UIBs) observed in many regions of the Interstellar Medium (ISM).

Since the suggestion of their presence in the Interstellar Medium (ISM) by A. Léger and J.L. Puget in 1984 [A&A137, L5 (1984)] to account for the origin of "unidentified infrared bands" (UIBs) this family of molecules has triggered a very large number of experimental and theoretical studies. The principle of the UV to IR conversion mechanism is a fast intramolecular internal conversion process, in which the electronic excitation is converted into vibrational quanta. However the experimental laboratory confirmation of this physical mechanism is extremely difficult since it requires to keep the molecules in collision-free conditions during milliseconds to seconds time intervals.

Simultaneously, extensive observation programs towards "reflection nebulae", thanks to appropriate instruments onboard of space missions like ISO, Akari and Spitzer, have been conducted since 1995, allowing to constrain in a better way the interpretation of these mid-infrared emission features: the AIB's (standing for Aromatic Infrared Bands) [Rosenberg, Berné, Boersma A&A, 566, L4 (2014)]. These regions of the ISM are acting like efficient light-converters from UV-VUV to mid-IR, but the actual nature (size, structure and charge state) of these IR-light emitters is difficult to derive from observations only.

The laboratory UV-VUV spectroscopy and photo-dynamics of PAHs in neutral and cationic forms are then essential to investigate and understand in detail the behavior of the *Astro-PAHs* in specific astrophysical conditions. Hopefully these results may then allow an informative comparison with observational data from space telescopes. Experimental as well as theoretical information about the PAHs structures, their formation mechanisms, reactivity, intramolecular conversion processes and their subsequent spectroscopic signatures are obviously of major interest.

A particular question concerning these *Astro-PAHs*, having received a quite important contribution from astrophysicists [see for instance "The Physics & Chemistry of the Interstellar Medium", by A.G.G.M. Tielens, Cambridge University Press, 2005, Chapters 3 and 6], involves their contribution to the heating of the ISM. The role of "hot" photoelectrons resulting from the photoionzation of very small graphitic grains or PAHs, has been put forward since the early paper by B.T. Draine [ApJ,ss, 36, 595-619 (1978)]. A number of other contributions discussing the

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"photoelectric heating" followed, among which: Verstraete et al, A&A, 237, 436 (1990); Bakes & Tielens, ApJ, 427, 822 (1994), Weingartner et al, ApJ.ss, 134, 263-281 (2001); E. Habart et al, A&A, 373, 702 (2001). These processes are also discussed in the context of the global dust spectral energy distribution [Compiègne et al, A&A, 525, A103 (2011)].

The ionization potentials (IP) of PAHs differ from a specific molecule to another, but their values remain in a limited range: from ~7 eV (for Nc > 40 Carbon atoms) to ~8 eV for Naphthalene (Nc=10). These values, remaining significantly below the Lyman cut-off at 13.6 eV, leave the possibility to produce energetic photoelectrons. On the other hand, the PAHs photoionization cross sections (usually considered to be proportional to the number of carbon atoms) get quite large near their maximum value [~ 33 Mbarn per C-atom, see Verstraete et al, A&A, 237, 436 (1990)] when photon energy (hv) gets around 17 eV. Consequently a significant part of the *Astro-PAHs* must be present in cationic forms, while an equivalent number of photoelectrons created by these single photoionization events are also present. Their kinetic energy is determined by the final cation states, as: KE = hv − (IP+ E_i) where E_i is the final vibronic energy of the cation. These fast photoelectrons could then transfer part of their kinetic energy (KE) to any collision partner available in the local ISM. This whole process (Fast photoelectron production + Collisional energy transfer) is responsible for the so-called photoelectric heating of the ISM, playing a pivotal role in the equilibrium of the interstellar models.

Thanks to the availability of the double imaging electron/ion coincidence spectrometer DELICIOUS3 set-up on the DESIRS VUV beamline at the SOLEIL synchrotron facility, we have conducted a systematic study to characterize in details the photoionization behavior of a series of nine PAHs, covering a broad size range (Nc =13 to 20) and differing in their structures (compact or not, presence of pentagons, methyl substituted, non-planar). For a majority of them we have also obtained information on the dissociative ionization channels (from one to three H-losses).

We confirm that the total VUV ionization yield (TIY) reaches a maximum, in agreement with the VUV absorption peak, which remains close to 18-20 eV for the parent PAHs, as well as for the dehydrogenated species.

The slow photoelectron spectra (SPES) of the whole series of PAHs have revealed the rich vibronic structures of the relevant parent cation excited states, as well as the appearance energies for de-hydrogenation (H-loss) dissociative ionization channels. The vibronic structures of the corresponding product species, have also been properly characterized.

Some major and global results of this extensive study will be presented and discussed.

The physical state of CO-dark gas in the perseus arm

Michael Busch[1*†], Ron Allen[2‡], Philip Engelke [1], Dave Hogg[3], David Neufeld[1], Mark Wolfire[4]

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We report the results from a new, highly sensitive ($\Delta T_{mb} \sim$ 3mK) survey for thermal OH emission at 1665 and 1667 MHz over a dense, 9 x 9-pixel grid covering a 1 square degree patch of sky in the direction of L = 105.00, B = +2.50 towards the Perseus spiral arm of our Galaxy. We compare our Green Bank Telescope (GBT) 1667 MHz OH results with archival CO(1-0) observations from the Five College Radio Astronomy Observatory (FCRAO) Outer Galaxy Survey within the velocity range of the Perseus arm at this galactic longitude. Of the 81 statistically-independent pointings in our survey area, 86% show detectable OH emission at 1667 MHz, and 19% of them show detectable CO emission. We explore the possible physical conditions of the observed features using a set of diffuse molecular cloud models. In the context of these models, both OH and CO disappear at current sensitivity limits, CO emission does not appear until the volume density exceeds 100-200 cm^{-3}. These results demonstrate that a combination of low column density and low volume density can explain the lack of CO emission at sightlines exhibiting OH emission. The 18-cm OH main lines, with their low critical density of n$^{*} \sim 1$ cm^{-3} , are collisionally excited over a large fraction of the quiescent galactic environment and, for observations of sufficient sensitivity, provide an optically-thin radio tracer for diffuse molecular hydrogen.

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Grain surface chemistry and its impact on the gas phase

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[2] LERMA – Observatoire de Paris, Université de Cergy Pontoise – France
[3] Centro de Astrobiologia (CAB, INTA-CSIC) – Madrid, Spain
[4] Laboratory for Astrophysics, Leiden Observatory, University – Leiden, The Netherlands
[5] Aix Marseille Universiteé, Marseille, France

Interstellar dust grains have been recognised to be important catalysts for the formation of the simplest (H_2) to the most complex molecules (amino acids) in space. While many processes occurring on dust surfaces have been studied experimentally and theoretically during the last decades, the step from experimental and theoretical studies to astrophysical modelling and observations still represents a great challenge.

I will present some of the important processes driving the chemistry on surfaces and discuss how such processes impact the gas phase. More precisely, I will concentrate on how the reactivity on surfaces can be responsible for the release of species in the gas phase as well as the process of accretion, which transforms gas phase species into solid species. Recent experiments or theoretical studies used to constrain these processes will be presented

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Carbon chemistry in evolved stars

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I will present the chemistry of carbon in C-rich evolved stars. The characterization of the molecular content of the ejecta of these objects has been obtained through sensitive optical, infrared and millimeter and submillimeter wave spectroscopic observations using the largest telescopes at all wavelengths. A view of the chemical content derived for these objects will be presented. The data gathered from these astronomical observations are the basic input for novel laboratory experiments within the framework of the Nanocosmos synergy project of the ERC. In these experimental setups, in particular in the stardust machine, we simulate at the best the physical and chemical conditions prevailing in the photosphere of evolved stars. The first experiments that we are going to present in this conference are related to the formation of carbon clusters and hydrocarbons as a first step to the formation of dust grains.

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Ices in small dense molecular cores

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The cold surfaces of dust grains in dense molecular clouds are chemical factories where simple and complex molecules are formed. The icy grain mantles promote grain growth and contain the building blocks of planetary systems. The conditions promoting complex molecule formation (e.g., density, time scales) are currently not well observationally constrained. We selected a sample of 16 stars behind five small ($\leq$2 pc in diameter) molecular clouds that we observed with IRTF SpeX simultaneously in the atmospheric L and M bands. We model the spectral type of the stars using the IRTF spectral library of giants and determine the baseline for H_2O and CO ice features at 3.1 μm and 4.67 μm, respectively. We also detected the 3.53 μm C-H stretching mode of CH_3OH ice in at least one of our targets. CO ice hydrogenation to H_2CO and CH_3OH ice are key initial steps in the formation of more complex molecules. We analyze the absorption band profiles to determine the ice mantle composition, in particular the relation between CO and CH_3OH ice. We also determine ice abundances. To put the ice formation scenarios into the context of the physical conditions (e.g., increased density is expected to be a key factor in CH_3OH formation), we have constructed very deep, high spatial resolution extinction maps for each cloud using photometry from UKIRT WFCAM JHK bands and Spitzer IRAC channels 1 and 2. We employ the latest techniques in extinction mapping using the XNICER routine (Lombardi, 2018). This work is in preparation for the large scale ice maps that will be obtained with the slitless spectroscopy mode of NIRCAM on JWST (part of a GTO program).

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Investigating interstellar dust in local group galaxies with new UV extinction curves

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It is well known that the standard Milky Way UV extinction curve does not hold even in the most nearby galaxies, the LMC and the SMC. It is not even known whether the standard curve holds throughout our own galaxy because our position in the disk of the Milky Way, where extinction is high, prevents us from seeing most of our galaxy at UV wavelengths.

We have a unique opportunity, while we still have the capability to obtain UV spectra with HST, to map out the UV extinction properties of interstellar dust across other nearby galaxies. We are engaged in a long term program to relate the properties of interstellar dust across a sample of Local Group galaxies with different global characteristics such as metallicity and star formation activity. We will present results from our recent HST programs, which obtained new STIS UV spectra of reddened stars in the SMC, M31, and M33.

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The importance of the atomic history in time-dependent simulations of the interstellar gas – from non-thermal to thermal distributions

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The majority of the numerical models of the interstellar gas include a sink term in the energy equation through a tabulated cooling function (either calculated in collisional ionisation equilibrium or in non-equilibrium ionisation conditions). These simulations do not trace the time-dependent atomic history of the gas parcels. Hence, it is assumed that all gas parcels have exactly the same atomic history, which of course is unphysical.

We present the latest developments in the subject pointing out the need for self-consistent calculations of the time-dependent dynamical and atomic evolution of the plasma and the consequences for the simulated emission in a large range of wavelengths. Our simulations include the ions of H, He, C, N, O, Ne, Mg, Si, S, Ar, and Fe in a total of 131 equations, plus molecular chemistry of H, C, and O. These calculations comprise the time-dependent MHD evolution of gases between the disk and halo with a unprecedented resolution of 0.25 pc.

We further look into the use of non-thermal plasmas with electron distribution functions which deviate from the Maxwell-Boltzmann distribution, and discuss the need of numerical methods able to track down the effects of these distributions in the plasma evolution. This work demanded the development of a plasma emission module taking into account all the processes associated with ionization, recombination, excitation, de-excitation, Auger effects, etc., and the calculation of the ionization states and levels populations in optically thin plasmas.

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Observing facilities for astrochemistry: evolution and future perspectives

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Progress in unveiling the Molecular Universe has gone hand in hand with the development of IR, mm and submm observing facilities and their instrumentation. In particular in the early days, where the NRAO 12-meter antenna played a key role, every progress in receiver performance, in frequency coverage and sensitivity, paid off immediately in more detections of molecules and better understanding of the physics and chemistry of the ISM components. Soon more antennas were constructed and the Molecular Universe became an important and challenging science case for a global community. In parallel to ground-based facilities, IR and submm space observatories came into existence. In particular the first cooled observatory, ISO and its spectrometers, showed the power of space IR spectroscopy for molecular and ionic line investigations. This was further exploited by Spitzer and even more by Herschel's spectrometers.
Meanwhile the combined efforts from ESO, NRAO and NAOJ, to get ALMA project defined, funded and constructed, has ultimately resulted in an incredible tool for Astro-Chemistry, with ultra-sharp images in every observed spectral line. ALMA's development program goals are to get even higher spatial resolution with wider IF bandwidths for more instantaneous spectral coverage. There is now also the successful airborne SOFIA facility with a FIR heterodyne spectrometer, be it with limited observing time and some hindrance of the atmosphere. Nevertheless, new space missions have been or are being studied and defined to complement ALMA, in particular in the FIR domain where many hydride and ionic lines provide a unique ISM toolbox. A follow up for Herschel needs higher sensitivity and better angular resolution. Within a few years we expect data from JWST's MIRI instrument and there is a good chance for a future large IR/FIR space observatory through SPICA, Millimetron and OST. Fortunately, one of them, Millimetron, will have heterodyne receivers with the required high (106) spectral resolution and with a 10-meter aperture. These missions and their capabilities, to keep providing Xander cs with the necessary data, will be addressed in this presentation.

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Unravelling dust nucleation in astrophysical media using a self-consistent, non-steady state, non-equilibrium polymer nucleation model for AGB stellar winds.

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Over 200 molecules and 15 dust species have been detected in the interstellar medium, stellar winds, exoplanets, supernovae, active galactic nuclei etc. One of the most fundamental questions in astrochemistry deals with the phase transition from simple molecules to larger gas-phase clusters and eventually dust grains. The outflows of evolved stars are the best laboratories to answer this pivotal question due to their rich chemistry and relatively simple dynamical structure.

Indeed, the winds of AGB and RSG stars have been recognized for a long time as key chemical laboratories in which more than 80 molecules and 15 dust species have been detected thus far. The general hypothesis of their mass loss mechanism is a combination of stellar pulsations and radiative pressure on newly formed dust grains. Through their winds, they contribute ∼85% of gas and ∼35% of dust to the total enrichment of the interstellar medium, and therefore are the dominant suppliers of pristine building blocks of interstellar material.

In the winds, a large variety of chemical reactions occur, including unimolecular, 2- and 3-body reactions, cluster growth and grain formation. However, current models simplify dust formation, which starts as a microscopic phase transition called nucleation. Various nucleation theories exist, yet all assume chemical equilibrium, growth restricted by monomers, and commonly use macroscopic properties for a microscopic process. Such simplifications for initial dust formation can have large repercussions on the type, amount, and formation time of dust. By abandoning equilibrium assumptions, discarding growth restrictions, and using ab-initio quantum mechanical properties, we have constructed and investigated an improved nucleation theory in AGB wind conditions for four dust candidates, TiO_2, MgO, SiO and Al_2O_3. To obtain the quantum mechanical properties, we have performed density functional theory (DFT) calculations, including a vibrational analysis, to determine the Gibbs free energy for all nucleating species.

We report the viability of these four candidates as first dust precursors and reveal implications of simplified nucleation theories. Assuming the monomers are present, we show that Al_2O_3 is the favoured precursor due to its rapid growth at the highest temperatures and as such is the only species that potentially can explain the detection of large transparent dust grain in the close vicinity of some AGB stars. However, when considering an initially atomic chemical mixture, only TiO_2-clusters form but at considerably lower temperature. Still, we believe Al_2O_3 to be the prime candidate due to substantial physical evidence in presolar grains, observations of dust around AGB stars at high temperatures, and its ability to form at high temperatures. We expect the missing link to be insufficient quantitative data of gas-phase reactions with Al atoms or Al-containing molecules.

We show how the recent ALMA Large Program ATOMIUM (113 hr) will allow elucidating the dominant chemical pathways in these winds, as such forming an observational testbed for constraining chemical kinetics modelling including pinpointing some of these missing reaction pathways. Some of these missing pathways are currently investigated, both using laboratory experiments and the RRKM theory to derive their reaction rates. We report on the newly obtained reaction rate coefficients and the impact thereof in chemical kinetics wind modelling.

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Formation of molecules on cold interstellar grains

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In 1982, Tielens & Hagen published an article entitled "Model calculations of the molecular composition of interstellar grain mantles" which is now cited 619 times (May 2019), as well as a companion article, signed Tielens, on deuteration effects.
Almost 40 years later, what progress has been made on the topic of the formation of molecular mantle on interstellar dust? Has the formalism of the model been reformed? Were the initial guess correct? Have new mechanisms been found?
During my presentation I would like to compare the proposals made in this founding paper, and the the last decade experimental studies about the mechanisms of molecule formation on dust grains. In particular, I will compare the formation of water and formamide initially proposed with what is known today. I will address the theme of diffusion and tunnel effect, which are central mechanisms from this founding study. We will then see what remains of this work and the considerable influence it has had on understanding the formation of ice mantles.
If time allows, I will finally show our latest results on hydrogenation and oxidation of coronene at low temperature.

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Astrochemistry of protoplanetary disks from an observational point of view

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The formation of planets together with that of comets and asteroids occurs through the combination of dust and gas lying within the disks surrounding young stars. This leads one to ask whether the properties of emerging planets along with their primitive atmospheres are shaped by the chemical composition of the disk.

Thanks to recent progress in instrumentation (i.e. high angular resolution and high sensitivity) for (sub)millimeter arrays, such as NOEMA and ALMA, new results about the origin of the material that might be incorporated into planets have been obtained. I will review some notable results on the detection of organic molecules towards protoplanetary disks along with that of S-bearing and carbon-chains species.

Finally, based on our recent ALMA observations of formic acid, I will show that complex organic chemistry is taking place in objects where planet formation occurs.

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The Orion bar: from ALMA images to new dynamic PDR models

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Far-UV photons (FUV, E < 13.6 eV) from hot massive stars regulate, or at least influence, the heating, ionization, and chemistry in many regions of the ISM. The Orion Bar, the prototypical strongly irradiated PDR, is illuminated by a FUV flux of few 104 times the mean interstellar radiation field. Because of its proximity and nearly edge-on orientation, the Bar provides an excellent template to investigate the chemical content, structure, and dynamics of an irradiated molecular cloud edge. In the last years, we have used ALMA to image a small field of the Orion Bar, where the transition from atomic to molecular gas takes place. These observations provide an unprecedented sharp view of this critical transition layer (< 1" angular resolution or <414 AU). The resulting images show the small-scale structure in gas density and temperature, as well as the steep chemical abundance gradients. The images suggest photo-evaporative gas flows and instabilities at the edge of the molecular cloud. These observations have triggered the development of new hydrodynamic PDR models that try to explain some of the most unexpected observational results, for example the apparent small separation between the H/H_2 and C^+/CO dissociation fronts and the high gas thermal pressures inferred in the molecular PDR. In this talk I will stress the dynamical and non-equilibrium nature of the interaction between UV radiation from young massive stars with their parental cloud. These questions are at the core of our understanding of stellar feedback, a collection of complicated processes that take place at many galactic scales and drive the evolution of the ISM.

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First astrophysical detection of the helium hydride ion (HeH^+)

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The helium hydride ion, HeH^+, has been detected in space for the first time with the GREAT spectrometer onboard the SOFIA. Through observations of its fundamental rotational transition at 2.010 THz, HeH6+ was detected toward the young planetary nebula NGC 7027.

This detection brings a decades-long search to a successful conclusion. I will review the history of the study of HeH^+, from its discovery in the laboratory almost a century ago to its recognition in the late-1970s as a potentially-detectable astrophysical molecule, and its role as the first molecular bond that formed when, 13 billion years ago, falling temperatures in the young Universe allowed recombination of the light elements produced in the Big Bang. At that time, according to models for the Early Universe, ionized hydrogen and neutral helium atoms reacted to form HeH^+.

The details of the SOFIA observations will be presented, and the implications of the measured line intensities will be considered in the context of astrochemical models. Follow-up studies toward other sources and through observations of other spectral lines will be discussed briefly.

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[CII] optical depth and self-absorption in M17SW

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M17 is one of the brightest and most massive star-forming regions in the Galaxy. It is located at 1.98 kpcs and the cloud is illuminated by a large young cluster (> 100) of OB stars. M17SW is located in the southwestern side of the M17 complex and contains the nearby UCHII region. It is considered as a prototype of an edge-on interface. The M17SW interface has a highly clumpy structure, proven by several studies of ionized, atomic and molecular emission. We have observed the [CII] 158 um fine structure atomic line at high resolution and S/N towards 7 selected positions in M17SW, using the SOFIA/upGREAT 7x2 array heterodyne receiver. The high S/N allowed us to detect the faint [13CII] hyperfine structure satellites around the [12CII] line. From comparisons between both isotopologues, we have detected that the [12CII] line is optically thick and heavily self-absorbed, this situation is in contradiction with the traditional view of optically thin [12CII] emission.

From there, we have performed a more complex and sophisticated analysis, with a multicomponent double layered model. We have assumed that the emission is emitted by a background layer, and absorbed by a foreground layer. This analysis allowed us to derive the physical properties of the $12C^+$ gas, namely the excitation temperature and column density of the gas. We have found that the background gas has really high column density, larger than expected from single layer PDR models, confirming a structure of clumpy and fractal dense clouds.

Also, we have found the existence of cold ionized and dense foreground gas visible in [CII] absorption that cannot be explained with any known source scenario for the moment.

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From astrochemistry to astrobiology? A few selected papers on cosmic ices evolution

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Interstellar dirty ices are observed in regions of star formation where disks, planets and various debris do form and evolve and where complex organic molecules are formed [1]. Thanks mostly to space borne observations such as those obtained from IRAS (1983), ISO (1995), and Spitzer (2003) —2-4], these ices are well documented. In molecular clouds, the presence of cold surfaces in a reducing H-rich environment, combined with the availability of abundant and "important for life" volatile elements (the so-called CHNOPS in the astrobiological community), lead to the formation of hydrides (e.g. H_2O, NH_3, CH_4) frozen on cold grains, as already suggested in the work of Oort and Van de Hulst as early as 1946 [5], bearing in mind that the same cold surfaces are essential for molecular hydrogen formation [6]. Two-body ion-molecule and neutral reactions, well studied in astrochemistry, will account for CO and derivatives but they will also end up, at least partially but unavoidably in ices (fig 4. of [7], the first model providing evidence for ice formation], where they will fully take part in the chemistry of the cosmic ices.
Astrophysical ices cannot escape energetic and thermal processing [12b] as suggested in a solar nebula model from Ciesla and Sandford [8]. This processing generates a largely unpredictable and complex solid state bulk chemistry, essentially from radical recombinations [9], even if two-body surface diffusion reaction chemistry was initially pioneered, in molecular clouds, in the early work of Tielens and Hagen [10]. This work was soon followed by the first tentative to empirically but successfully include some photochemistry using the CO2 molecule as a possible marker [11]. Indeed, these processes may be approached in the laboratory using conventional tools of matrix isolation techniques [12] and presented in detail in Karin Oberg's comprehensive work [12b].
If ice simulations have been fruitful in the 95-05's decade to decipher and interpret ice compositions from infrared spectroscopic data alone (see [13, 14] as examples), templates of organic materials generated by this chemistry are now routinely studied by ex-situ techniques. Extensive use of sophisticated analytical chemistry methods, either targeted, such as gas and liquid phase chromatography/mass spectrometry (GC-LC-MS), or non-targeted, as with very high resolution mass spectrometry (VHRMS), as well as many other techniques, partly borrowed from cosmochemistry, the science of meteorites. They allow for a full analytical survey of the molecular organic diversity and complexity observed in these laboratory ices and, by extrapolation, to cosmic ices and possibly to meteorites. The goal is to characterize the organic matter that is produced and generically called, in the laboratory, organic residues [14b] (soluble as well as insoluble as it is the case in primitive chondrites). As a matter of fact these studies may help bridging the gap between astrochemistry and cosmochemistry by allowing a true bottom-up approach to the organic diversity observed in small bodies of the Solar System and in particular in meteorites [15] and now recently in micrometeorites [16].
Concentrating, in this short review, on the soluble part of this material, many interesting molecules, often too quickly referred as "molecular bricks of life", are now routinely detected such as a wealth of amino acids [17, 18], including complex precursors of peptidic nucleic acids (PNA) [19], nucleobases [20], dipeptides[21], a collection of aldehydes and sugars up to ribose [22] and deoxyribose [23] and, very recently phosphorylated compounds, when native phosphorus is implemented in the original ices [24, 25] as suggested by some observations on comet 67-p by the Rosina instrument on the comet probe Rosetta [26]. All these compounds, many of them indeed present in meteorites while others await a positive detection, reinforce the hypothesis on the potential importance of exogenous delivery of key organic compounds at the surface of telluric planets for the onset of prebiotic chemistry [27], prior to the

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emergence of life.

It is remarkable to note that, up to now, only one chiral molecule is observed in the gas phase by radio astronomy [28]. This can be understood by the fact that, in order to obtain chiral molecules, where one carbon atom is fully asymmetric (bonded to four different chemical groups) actually implies quite complex molecules that are indeed abundant and diverse in primitive chondritic meteorites. Enthralling results have shown that, from the achiral ices in the laboratory, submitted to circularly polarized ultraviolet light from a synchrotron source, the ice evolution naturally leads to the formation of chiral molecules within the residues. Chiral ultraviolet photons are thus able to generate symmetry breaking in amino acids within the ice-residue organic template [29,30], a characteristic that is indeed observed in some meteoritic amino acids found in meteorites [see [31] for a review). Note that 97 amino acids are observed in Murchison, all basically chiral. The presence of CPL in regions of star formation is now firmly established [32-34], suggesting a possible connection between ice processes and the origin of enantiomeric excesses in chondritic meteorites. A scenario may be proposed following the model of the solar nebula [8].

Finally, a word of caution should be brought into the debate as far as astrobiology is concerned. Molecular bricks of life should be understood as plainly dead molecules and do not possess any characteristics attributed to living systems even minimal ones. What is proposed in this review is a general and holistic description of the evolution of cosmic ices from molecular clouds to organic matter in our Solar System as, for example, described in [35]. Clearly enough, some (yet unknown?) conditions for the emergence of a prebiotic chemistry leading to minimal life on a telluric planet should be met. That is clearly out of the scope of this rather uncomplete review, however with may be a couple of questions to bear in mind for the reader: (i) what is the final fate of this organic matter in a given environment, in particular in a far-from equilibrium chemistry? And (ii) can this evolution be somewhat approached in the laboratory in a comparable holistic manner as the one presented for the chemical evolution of dirty ices? That is clearly the next experimental step toward astrobiology.

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Xander Tielens and his contributions to understanding the ISM

David Hollenbach[1*†]

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This talk highlights aspects of Xander Tielens' career from graduate student at Leiden University in the late 70's to his current professorship at Leiden.
These highlights include his tenure at NASA Ames, his involvement with infrared astronomy and laboratory astrophysics, his management roles in SOFIA and Herschel, and some recent honors including the Spinoza Prize in 2012.
The Conference includes five main topics: PDRs, PAHs, Ice, Dust Life Cycle, and Astrochemistry. I briefly discuss a few of Xander's contributions to these topics.

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Experimental studies of the catalytic role of oxygen functionalized PAHs

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In cold regions of the interstellar medium (ISM) siliceous and carbonaceous dust grains are covered by an icy mantle with the most dominant component of the ice being H_2O. Polycyclic Aromatic Hydrocarbon (PAH) molecules along with other simple and complex molecules are also expected to condense onto the dust grains. Laboratory processing of water ice and PAH mixtures with energetic radiation such as UV light or protons show that superhydrogenated PAHs are produced alongside PAHs with alcohol and ketone functional groups indicating that such species are formed in the ISM on icy grains [1] [2]. Interstellar ices could contain neutral and ionized PAHs, alcohols, ketones and quinones at the 2% - 4% level relative to water [3]. Functionalized PAHs are of both astrochemical and astrobiological significance and their interaction with abundant atoms in the ISM is yet to be well characterised.

In photodissociation regions of the ISM where UV photons dissociate molecules and grain surface reactions are less efficient, PAHs were postulated as catalysts for molecular hydrogen formation. Experiments and theoretical calculations indicate that superhydrogenated PAHs [4],[5] provide a route towards H2 formation though the impact of the presence of other functional groups on such routes remains unclear. Laboratory studies of a variety of PAHs based on their size, functionalization and edges is key to identifying specific PAH molecules in the ISM. I will present laboratory studies of the catalytic activity of functionalized PAHs, in particular, the catalytic role of 6,13 – pentacenedione (PQ) in the formation of molecular hydrogen along with other small molecules like OH and H_2O.

Surface science techniques provide a means study neutral PAHs. We prepared a monolayer of PQ under ultra-high vacuum conditions on a HOPG surface mimicking a carbonaceous dust grain and exposed it to a controlled fluence of hydrogen atoms. The surface was then heated in a controlled manner while the products were collected in a quadrupole mass spectrometer. This technique, known as temperature programmed desorption, provides us with valuable information concerning the reaction kinetics through mass spectrometry from which we can also extract reaction cross sections.

The experimental data demonstrates the formation of superhydrogenated PQ species. Specific superhydrogenation degrees are found to be more stable than the others resulting in magic numbers in the hydrogenation sequence. Such magic numbers indicate barriers to addition as observed in experiments with coronene and pentacene [6]. Importantly, the first species to form even at very short H atom exposures has a mass of 294 amu indicating the loss of an oxygen atom from PQ, potentially through the formation of H_2O or OH. DFT calculations are required to support the prominent masses observed for intermediate H atom exposure and to determine the route of loss of oxygen atoms. The reaction cross section was determined and is at least 10 times higher than those measured previously for coronene.

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Astro-PAHs: a journey from space to the laboratory

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The presence of polycyclic aromatic hydrocarbons (PAHs) in astrophysical environments has been proposed to account for the aromatic infrared bands (AIBs), a set of mid-infrared emission bands, which are triggered by the absorption of ultraviolet (UV) photons [1,2]. Due to their interaction with the UV radiation field, astro-PAHs play a key role in the physics and chemistry of photodissociation regions at all scales, from protoplanetary disks to galaxies. Underlying processes include the heating of the gas by photoelectric effect [3], the extinction of UV photons [4], and the formation of H_2 [5].

The AIBs arise from hot molecules, which makes it difficult to perform a detailed spectral identification. No match between features of the electronic spectra of cold PAHs and the diffuse interstellar bands (DIBs) [6] has so far been reported. Only fullerene, C_{60}, and its cation, C_{60}^+, could be identified in AIB [7-9] and DIB spectra [10]. Astro-PAHs have been shown to evolve under UV processing [11], which could lead to the formation of C_{60} [12]. The unprecedented capabilities of the coming James Webb Space Telescope should bring further observational insights into these aspects. On the laboratory side, we are gaining a better knowledge on the dynamics of ionisation and dissociation of PAHs upon interaction with UV photons [13-15] as well as on the kinetics of radiative cooling [16].

The formation routes of astro-PAHs and fullerenes are another key issue to be elucidated. The scenario of gas-phase condensation in the shells of evolved stars has been discussed following experiments using laser ablation, combustion, laser pyrolysis, or cold plasmas [17-20]. Experiments using the sophisticated Stardust machine [21] together with cold plasmas [22] are now ongoing in the framework of the Nanocosmos ERC Synergy project [23]. The evolution of the molecular content with the experimental parameters is tracked with the AROMA setup [24] and compared with the composition of meteorites.

The success of the astro-PAH field can be attributed to the pioneers of the interstellar PAH hypothesis although it has now likely overpassed their expectations. Driven by laboratory astrophysics, the field keeps expanding and involves a large interdisciplinary community, including observers, experimentalists, theoreticians and modellers to solve the chemical and photo-physical specificities of astro-PAHs.

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PDRs near and far: the extraordinary utility of photodissociation region models

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The first PDR models are nearing 40 years old, and the utility of these models continues to expand. Recently, models have been applied to observations of regions as diverse as: nearby diffuse and translucent clouds; dense star forming regions; the Galactic Center and outer disk of the Milky Way; and star-forming galaxies at high redshift. I will review some representative cases, highlight some potential pitfalls, and discuss current and future efforts with ALMA and SOFIA.

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The PROduction of Dust in GalaxIES (PRODIGIES)

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My research group is organized around the central theme of the PROduction of Dust In GalaxIES (PRODIGIES), in part building on the success of the SAGE collaboration, in which Xander was a key collaborator. SAGE focussed on the life cycle of dust in the Magellanic clouds, and one of the main results from that collaboration was the apparent mismatch between the dust production seen in the ensemble of evolved stars and the dust reservoir in the interstellar medium. Apparently, at the present rate of dust formation, replenishment of the dust reservoir in the ISM of the LMC would take 35 Gyr, longer than the age of the LMC, and indeed the Universe itself. Thus, the so-called "dust-budget crisis" (e.g. Rowlands et al. 2014) is not just confined to the high-redshift universe, but has a local analogue as well. In PRODIGIES, we investigate different aspects of the dust production in galaxies. For instance, we recognize the limitations of estimating the dust production by evolved stars using mid-infrared photometry only, and are currently conducting a volume limited survey of evolved stars in the Solar Neighborhood (the Nearby Evolved Stars Survey: NESS) to establish the mass-loss history of individual stars, including the gas and dust masses, measured in the submillimeter, using single-dish facilities like the JCMT, APEX, and Nobeyama, as well as the SMA and the ALMA-ACA. We also look at the other side of the equation, and are investigating uncertainties and systematic errors that occur in dust mass measurements in the interstellar medium, which rely on far-infrared and submillimeter opacities. In active galaxies, the central AGN is a potential source of dust, and we have investigated the mineralogy seen in the freshly produced dust in these kind of environments. It is established that a large range of dust compositions is found in these environments, making it unlikely that the dust composition is universally the same in external galaxies, placing further doubt on the widespread use of a standardized dust model based on Galactic ISM measurements to establish the dust masses and other properties in external galaxies, near and far.

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Tracing PAH size in prominent nearby mid-infrared environments

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We present observations from the First Light Infrared TEst CAMera (FLITECAM) on board the Stratospheric Observatory for Infrared Astronomy (SOFIA), the Infrared Array Camera (IRAC) and the Infrared Spectrograph (IRS) SH mode on board the Spitzer Space Telescope in three well-known Photodissocation Regions (PDRs), the reflection nebulae (RNe) NGC 7023 and NGC 2023 and to the South-East of the Orion Bar, which are well suited to probe emission from Polycyclic Aromatic Hydrocarbon molecules (PAHs). We investigate the spatial behaviour of the 3.3, 7.7- 8.6, and 11.2 micron PAH emission bands and their ratios of 11.2/3.3 and (7-9)/11.2 which we use as an approximate measure of the average PAH size and PAH ionization respectively. We find that the relative PAH ionization increases with decreasing distance to the illuminating source in both RNe.

We further report that the average PAH size is at a minimum at the PDR front and increases inwards towards the illuminating source in both RNe. In addition, the average PAH sizes derived for NGC 2023 are greater than those found for NGC 7023 at all points. Both results indicate that the average PAH size depends on the radiation field intensity.

These results thus provide additional evidence of a rich carbon-based chemistry driven by the photo-chemical evolution of the omnipresent PAH molecules within the interstellar medium. In contrast, we did not detect a significant variation in the average PAH size found in the region South-East of the Orion Bar and report a peculiar PAH ionization radial profile.

These inconclusive results along with the complex morphology of this region beyond the initial edge-on PDR suggest a more in depth investigation into the photo-chemical evolution of this PAH population is required.

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Molecular complexity in solar-type star forming regions

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In 2003, Cazaux et al. presented the first inventory of complex saturated organic molecules around a low-mass protostar. With this work, the path to a systematic exploration of the chemical composition of solar-type objects was opened. Thanks to the advances in radioastronomical instrumentation, the Herschel space mission and the new generation of (sub)millimeter interferometers ALMA and NOEMA, it has now become possible to investigate the evolution of matter during the long process that brought it from prestellar cores to protostars and their disks, and eventually to the bodies of the Solar System.
Large observational efforts are being conducted with the IRAM and ALMA observatories to address this question. In particular, the IRAM ASAI and SOLIS Large Programs are investigating the gas chemical composition in the different stages a solar-type star undergoes during its formation. My presentation will highlight the main results coming out of ASAI and SOLIS, and will how they contribute to our understanding of our "chemical origins".

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The low-metallicity ISM of dwarf galaxies: the multiphase structure and the CO-dark gas

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While CO is the usual tracer of the H_2 reservoir in galaxies, it is challenging to detect in metal-poor galaxies,inspite of the rigorous star formation often taking place. The reduced dust abundance and hard UV radiation photodissociations the CO core leaving a large photodissociation region where the FIR fine structure lines emits from. In this zone the H_2 can be self-shielded from photo-dissociation. The FIR fine structure lines along with photodissociation and photoionisation models can be used to trace this reservoir of CO-dark molecular hydrogen. To quantify this reservoir we model the multi-phase ISM of the Spitzer and Herschel Dwarf Galaxy Survey with one goal of pinning down the total H_2 in a wide range of low metallicity environments. We also uncover the structure of the ISM of dwarf galaxies, notably the filling factor of the photodissociation and ionised gas components.

We find an important reservoir of molecular gas, not detected by CO, but residing in the C^+ - emitting reservoir, which may be the dominant molecular hydrogen component of low-metallicity star-forming galaxies. We suggest a general recipe to quantify the total mass of in galaxies, taking into account the CO and [CII] line intensity.

By exploiting the full suite of valuable MIR and FIR lines obtained from Herschel and Spitzer spectroscopy we are able to characterise the properties of the evolving ionized and neutral gas phases of galaxies, determine robust star formation rate tracers, ISM porosity and photoelectric heating efficiencies - some of the processes that shape a galaxy. With the future JWST, SPICA, and OST missions, we will be able apply the same methodology to the multiphase analyses of high-z galaxies.

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Damaged water ice: an opportunity for reactivity?

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The importance of on-grain processes towards reactivity in the interstellar medium (ISM) is still a matter of controversy. The role of water ice, one of the most abundant solid in the ISM, as catalyst may be manifold. One remarkable feature of water ice mantles is that it is subject to intense irradiations resulting in permanent destruction. We propose to take this into account. We present the typical case of the formation of formamide which has already been under scrutiny of several studies as a prebiotic molecule, see for instance [1,2,3]. The reactants HCN/HCN are adsorbed on damages water ice. Different pathways are considered by means of quantum mechanics modelling. Both cluster and periodic approaches are used. Drawbacks and advantages of each approach are discussed with a pragmatic tone.

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PAHs on/in water ice: structures, energetics and spectra from FTIR experiments and a multi-method theoretical study

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Polycyclic Aromatic Hydrocarbons (PAHs) are believed to be a significant reservoir of carbon in the interstellar medium (ISM) and have been proposed to be the carriers of the Aromatic Interstellar Bands (AIBs), a set of infrared (IR) emission bands observed in the [3 - 15 μm] range in many regions of the ISM. In dense environments, PAHs are likely to condense onto or integrate into water ice mantles covering dust grains and to contribute to the complex grain chemistry [1]. Understanding the role of ice in the processes involving adsorbed PAHs is therefore a key issue in astrochemistry. Another issue is the precise structure of interstellar ice, which remains unclear, although it is generally agreed that it is amorphous upon formation.
Our joint theoretical (classical molecular dynamics/force field simulations and SCC-DFTB calculations) and experimental (matrix isolation/solid phase FTIR spectroscopy) study has given rise to several conclusions, namely: we have demonstrated the role of water clusters [2] and of the ice structure [3] on the photo-reactions of PAHs with water ice ; a direct correlation has been shown between the location of energetically favorable adsorption sites and the presence of dangling OH (dOH) bonds ; and finally, a relationship between interface structures (number of interacting dOH) and vertical ionization potential (VIP) variation has been established [4]. Here, we will present evidence of how the surface of amorphous solid water (ASW) is perturbed by the adsorption of PAHs, leading to a redshift and a broadening of the dOH ice spectral feature [5]. We will also present a complete description of PAH-ice interaction in the ground electronic state at low temperature, providing the binding energies and barrier heights necessary to the on-going improvement of astrochemical models [6]. The influence of ice on the VIP of PAHs will be discussed, together with its astrophysical implications.

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Adsorption of volatile molecules on interstellar carbonaceous dust analogs

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The adsorption of molecules on the surface of dust grains is crucial for the physics and chemistry of interstellar clouds. Binding, diffusion and reaction of these molecules are determinant for the chemical inventory in many astronomical environments including comets, trans-neptunian objects and icy moons in the solar system. Interstellar grains consist mostly of silicates and carbonaceous materials with a small amount of metal oxides, carbides and sulfides. The surfaces of these refractory grains provide sites for adsorption and reaction. It is estimated that nearly 100% of Si, Fe and Mg, 30% of O, and 70% of C in the interstellar medium are locked in the grains [9]. In the diffuse medium, carbonaceous dust produces a characteristic absorption band at 3.4 mm attributed to hydrogenated amorphous carbon (HAC). The H/C proportion and the aromatic/aliphatic ratio in interstellar HAC remain controversial [4]. In the cold (< 20 K) interior of dense cores atoms and molecules freeze out on grain surfaces, forming ice mantels. Water is by far the most abundant component of these mantels, but CO_2 and CO are also present in relatively large amounts, CH_4 and NH_3 have also be detected and other species like N_2 and O_2 are assumed. Heating of the grains in the course of the cloud collapse that leads to star formation activates both chemistry and desorption. In the outer regions of a forming star, volatile species can be retained on the grains and then incorporated to larger bodies like asteroids, planets and moons.

Desorption studies, relevant for astrophysical conditions, have been carried out previously for surfaces of water-ice, graphite, graphene and silicates [1, 2, 3, 5, 6, 7, 8]. In this work we extend these studies to HAC surfaces taken as analogs of interstellar carbonaceous dust. To our knowledge this investigation has not been performed before.

Our experiments are designed as a two steps process. First we generate different HAC samples through deposition on Al substrates in RF plasmas of suitable precursors (CH_4, C_2H_2). In the second step we transfer the substrates with HAC deposits to our ultra-high-vacuum chamber and place them in the cold head of He cryostat. We then introduce volatile species (CH_4, CO, CO_2 or N_2) into the chamber trough multichannel arrays and deposit them on the HAC samples at selected temperatures down to 15 K. We take reflection absorption IR spectra (RAIRS) and perform line-of-sight thermal programmed desorption (TPD) to determine binding energies. The presence of two kinds of adsorption sites, likely associated with the HAC aliphatic and aromatic components respectively, will be discussed. This discussion will be supported by density functional theory (DFT) calculations of the adsorption energies of the volatile species on theoretical analogues of HAC. Comparison with previous literature data shows that volatile molecules are best retained by carbonaceous solids than by water-ice or silicate surfaces.

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Radioastronomical observations of PAHs and other aromatic species at the earliest stages of star formation

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Motivated by our discovery of benzonitrile (cyanobenzene; C_6H_5CN) in the dark cloud TMC-1, we have undertaken two large observational follow-ups with the GBT: GOTHAM and ARKHAM. Here, I will present the first science results of both projects. GOTHAM aims to explore the extent of aromatic chemistry in TMC-1, where we detected C_6H_5CN, using a deep spectral line survey; our detections of new interstellar molecules from this work will be described. ARKHAM seeks to understand how widespread detectable aromatic chemistry is at the earliest stages of star formation. We will also present our detections of benzonitrile in sources outside TMC-1, including those in which collapse toward protostellar formation, and a protostellar source itself, are included.

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The life cycle of dust in galaxies

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The life cycle of dust in galaxies touches all aspects of galaxy evolution and has moved into the main stream of galaxy evolution models. In this review talk, I will cover the key stages of this life cycle: dust production by dying stars, dust destruction in the interstellar medium by star formation (astration) and supernova shock waves, and growth of dust in the interstellar medium.

I will review recent work on this topic and discuss the promise of new and future observatories for this topic.

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SPHEREx: Surveying the Milky Way in biogenic ices

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IR absorption spectroscopy and submm emission-line spectroscopy suggest that ices are present within cold, dense (T $\leq$ 20 K; n$\geq$ 10^3 cm^{-3}) regions shielded from external UV radiation, including the mid-plane of planet-forming disks. Key biogenic molecules, such as H_2O, CO_2, CO, and CH_3OH, are locked into ice in variable, but large amounts, far exceeding that in the gas phase. In the case of H_2O, within these regions more than 99% is likely in the form of ice. It is becoming increasingly clear that ices play a major role in planetesimal formation within disks, and that ices are the source of water and organic molecules for newly forming planets. However, basic questions remain unanswered. For example, how do ices evolve from translucent to dense molecular clouds, and is the ice composition within protoplanetary disks inherited from the interstellar medium, or is it altered significantly within disks. To make further progress, we need to understand the abundances and composition of ices in all phases of star and planet formation. SPHEREx, the Spectro-Photometer for the History of the Universe, Epoch of Reionization and Ices Explorer, is a recently-approved NASA Medium-Class Explorer mission designed to: (1) investigate the distribution and abundance of water and biogenic ices in molecular clouds, young stellar objects, and protoplanetary disks throughout the Milky Way; (2) constrain the physics of inflation by measuring the three-dimensional distribution of more than three hundred million galaxies; and, (3) explore the origin and evolution of galaxies through a deep multi-band measurement of large-scale clustering. To achieve these goals, SPHEREx will obtain 0.75 – 5.0 μm spectra within every $6.2'' \times 6.2''$ region over the entire sky, or a total of 13.9 billion spectra. It implements a simple instrument design with a single observing mode to map the entire sky four times during its nominal 25-month mission. Launch is expected in 2023. SPHEREx will increase the number of currently available ice-rich absorption spectra (only about 200) by 100-fold, to a minimum 20,000 spectra toward interstellar clouds and disks of all types. Doing so, it will resolve long-standing questions about the abundance and evolution of such biogenic molecules as H_2O, CO, CO_2, OCS, and CH_3OH across the early phases of star and planet formation. It will operate from a sun-synchronous, low-Earth (600 km) orbit from which its $3.5^{\odot}\times 11.3^{o}$ total field of view will sweep out coverage circles on the sky. Every six months, SPHEREx will observe the entire sky. SPHEREx observations of the Galactic plane will be used for the ice investigation described here. SPHEREx coverage of the extragalactic sky – i.e., Galactic latitudes beyond $\pm \sim 10^{o}$ – will be used to refine our knowledge of cosmic inflation. SPHEREx's many overlapping, deep observations of the north and south ecliptic poles, which will be observed every orbit, will be used to constrain the cosmic history of galaxy formation. Bands 4 – 6 are of particular interest to the ices investigation due to the presence of important ice absorption features between 2.5 μm and 5.0 μm. Suitable background sources against which ice absorption spectra can be obtained have already been catalogued at 3.4 μm and 4.6 μm by the NASAWidefield Infrared Survey Explorer (WISE) mission. We estimate that SPHEREx will yield a transformative 1 – 2 million sources with high-quality ice absorption spectra, based on the more than 70 million catalogued WISE sources within $\pm 5^{o}$ of the Galactic plane that: (1) are spatially isolated; (2) show evidence of intervening gas and dust (derived from 2MASS+WISE data); and, (3) are sufficiently bright to yield signal-to-noise ratios of at least 100 per spectral resolution element, $\Delta\lambda$. By obtaining a 100-fold increase (or more) in available spectra, and by revealing the threshold optical depths at which ices form, SPHEREx will substantially advance our understanding of how ices build up and evolve as gas and dust progress from diffuse to dense clouds to circumstellar envelopes and, ultimately, protoplanetary disks. This talk will present an overview of the SPHEREx mission and its expected impact on the study of interstellar ices.

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ISM spectra from near- to mid-infrared

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This presentation reviews variations of the PAH emission in Galactic objects and nearby galaxies using the recent data from near- to mid-infrared. The Infrared Camera (IRC) onboard AKARI provided low-resolution spectroscopy in the near-infrared (2.5 - 5μm).

This spectral range was not covered by Spitzer/IRS, but contains the 3.3μm aromatic C-H and 3.4μm aliphatic C-H bands as well as several ice absorption features, providing useful information on PAHs and interstellar ices. Combining IRC and IRS spectra, full PAH spectra from nearto mid-infrared can be studied. In particular, the emission bands at 3.3 - 3.5μm are sensitive to the PAH size and the aliphatic to aromatic component ratio, whose information cannot be easily obtained solely from mid-infrared spectra. Analyses of objects that have been observed both with the IRS and the IRC are presented and the variation of properties of the band carriers, including the size and the fraction of the aliphatic component, is discussed. The IRC also had the imaging capability to observe the SED of the diffuse emission from near- to midinfrared (3 - 24μm) continuously.

This allows us to study the relative variation of the abundance of PAHs and very small grains in various environments. These data provide significant information for the study of processing of small dust species and ice components in the interstellar medium.

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Laboratory investigations on the chemical and optical properties of interstellar ice analogs

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The presence of icy mantles on dust grains in the line of sight to dense molecular clouds is clearly evidenced by infrared observations. Ices have been observed towards both low- and high-mass young stellar objects as well as towards quiescent dense clouds. In these environments ices suffer from energetic processing (i.e. ion bombardment and UV photolysis). Fast ions (keV-MeV) passing through molecular solids release their energy to the target along the ion track. As a consequence molecular bonds are broken and in a very short time (one picosecond or less), radicals and molecular fragments recombine giving rise to molecular species not present in the original sample. In the case of UV photolysis the energy is released to the target material through single photo-dissociation or ionization events per incoming photon. Laboratory experiments have shown that energetic processing modifies the chemical composition as well as the structure of thin icy films. Here I will present some results obtained in the Laboratorio di Astrofisica Sperimentale at INAF-Osservatorio Astrofisico di Catania (Italy). These investigations are aimed to study the chemical modifications induced by low-energy cosmic rays (keV-MeV) on interstellar ice analogs and to collect infrared spectra of relevant mixtures for the comparison with astronomical observations (ISO, Spitzer and in the near future JWST). However a direct comparison between spectra of thin films and spectra of icy grain mantles is not always possible. In fact, it is well known that particle shape and size can have very important effects on the profile of icy absorption features. The difference between bulk spectra and small particle extinction spectra depends on the optical constants (n, k) of the sample. From the knowledge of the optical constants, Mie-scattering calculations can be carried out. These show that absorption features of small particles can be shifted with respect to laboratory (bulk) spectra of thin films and subpeaks appear. If in principle optical constants can always be measured, in practice this is not straightforward especially in the case of mixtures and of irradiated samples. We developed an experimental method to know whether particle shape and size would affect the profile of an absorption feature and hence whether laboratory spectra of thin films are representative of small particles extinction spectra.

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H_2 and HCO· formation at the interface with crystalline models of icy mantles: insights from periodic DFT-MD simulations

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About 200 molecules have been observed in the interstellar medium (ISM), of which all those with more than five atoms contain carbon. Although this has been known for decades, astrochemists have been struggling for decades to understand what are the processes responsible for the observed richness of organic chemistry in space. The most popular models assume that everything happens on the interstellar grain surfaces.

Experiments provide some support to this paradigm, but since reproducing the interstellar conditions is extremely challenging, the suggested/assumed chemical processes need to be understood at the atomic level. Accordingly, periodic molecular dynamic (MD) simulations have been carried out at PBE-D3/TZVPP level with the CP2K code using the (010) crystalline ice surface as a model of icy mantels.

On this surface we studied the formation of the H_2 molecule, which is a fundamental process occurring on interstellar icy mantles, as well as the HCO radical formation (CO is the second most abundant species in the ISM), which is one of the most important precursor for the formation of many molecules (formamide, methanol, formaldehyde, formic acid, etc.), which, in turn, are the precursors of molecules of biological interest.

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Unravelling spectral signatures and photochemical processes of polycyclic aromatic hydrocarbons

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We present combined experimental and theoretical studies of spectral signatures and photochemical processes of neutral and ionic PAH species. We investigated PAH neutral molecules as possible carriers of the Diffuse Interstellar Bands (DIBs). We measured the high-resolution gas-phase electronic UV/VIS spectra of jet-cooled neutral PAHs and used these to validate vibrationless electronic transition calculations [$1a, 1b$].
The measured spectra show very strong vibronic coupling and the predictions were found to agree with the measured S1electronic states within roughly 1%, paving the way to narrow down on the identification of possible neutral PAHs as DIB carriers. We also investigated PAH ionic species as possible sink for missing deuterium in the universe [$2a, 2b$]. We studied the mechanism at play in the UV photolysis of several PAH isotopologues and recorded their fragmentations patterns as well as their IR spectra. The photolysis was found to incite a scrambling mechanism prior to fragmentation, locking deuterium to aromatic positions and preferably releasing hydrogen atoms, thereby leading to D enrichment of PAHs.

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The physics and chemistry on the surface of cosmic dust grains

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Dust grains play a central role in the physics and chemistry of practically all astrophysical environments. They influence the thermodynamic properties of the medium, provide a surface for chemical reactions responsible for the synthesis of a major part of important astronomically relevant molecules, and are building blocks of planets. Knowing the properties of grains, we can follow their pathways to larger astronomical bodies and trace back the history of planetary systems. Studies of physical-chemical processes on the surface of cosmic grain analogues lead to a better understanding of routes of the formation of complex organic molecules (COMs) and help to explain their detection and abundances in interstellar and circumstellar environments. In our recent laboratory experimental studies, we have shown a strong influence of the surface properties of nm-sized silicate and carbon grains, analogues of cosmic dust grains, on the formation and desorption of molecules. An alternative route of COM formation - grain surface processes - has been probed experimentally. Our results demonstrate, for the first time, that the bombardment of carbon grains by O and H atoms at low temperatures causes the formation of CO molecules, with their further hydrogenation leading to the formation of solid formaldehyde, a precursor of methanol. For the first time, we have put in evidence the catalytic role of the dust surface using the $CO_2 + 2NH_3 \rightarrow NH_4{+}NH_2COO$- thermal reaction on the surface of silicate and carbon grains. Surface catalysis on grains accelerates the kinetics of the reaction studied at the temperature of 80 K as compared to molecular solids. In the first laboratory study of the temperature-programmed desorption of water ice mixed with amorphous carbon and silicate grains, we have shown that the kinetics of desorption of H_2O ice depends strongly on the dust/ice mass ratio indicating the desorption of water molecules from a large surface of fractal clusters composed of grains. In addition, it has been shown that water ice molecules are differently bound to silicate grains in contrast to carbon. The photodesorption yield for H_2O molecules on carbon grains is noticeably higher as compared to silicate grains. This result could be explained by the hydrophobic surface properties of the carbon grains and a stronger absorption of UV photons by carbon increasing the surface temperature. A trapping of water ice molecules on silicate grains above the desorption temperature of H_2O has been detected. Trapped water can survive the transition from cold star-forming regions to accretion disks and stay in silicates in the terrestrial planet zone.

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Dust grain size distribution across the disc of spiral galaxies

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The physical properties of the dust are directly linked to those of the ISM where it is located. The dust is not only heated by the ISRF but it is also affected by other mechanisms that lead to a change in the physical properties and/or to the destruction of a particular dust grain type. These mechanisms dominate the evolution of the dust content as well as the grain size distribution in galaxies. Following [3] the main mechanisms are: (i) dust supply from stellar ejecta (AGB stars and SN), (ii) dust destruction via sputtering in SN shocks in the ISM, (iii) grain growth via accretion of metals in the gas phase, (iv) grain growth via coagulation, and (v) grain disruption/fragmentation (shattering) in SN shocks. All these processes act differently on large and small grains: (i) SNe and AGB stars are predicted to supply mainly large grains ([5, 10]), (ii) dust destruction by sputtering affect both large and small grains, (iii) grain growth via accretion is favoured when the number of small grains is large, as small grains have a larger surface-to-volume ratio [2]; (iv) grain growth via coagulation occurs in the dense ISM and move the grain size distribution towards larger grain sizes [8], and (v) fragmentation associated to shattering creates a large number of small grains [6]. Due to all these processes, the dust grain size distribution in a galaxy evolves with time. Therefore, the relative abundance of the dust grain types gives us very useful information to study the mechanisms that affect the dust evolution, which in turn is directly linked to the evolution of galaxies.

In this talk I present a detailed study of the relative contribution of the different dust grain sizes in a set of spiral galaxies: M33, NGC628 and M101. We have fitted the dust spectral energy distribution in a pixel-by-pixel basis across the disc of M33 [9] and M101 and NGC 628 [11]. We have used the classical Desert et al. (1990) dust model, which consists of three dust grain types: polycyclic aromatic hydrocarbons (PAHs), very small grains (VSGs) of carbonaceous material, and big grains (BGs) of astronomical silicates. We have applied a Bayesian statistical method to fit the individual SEDs and derived the best output values from the study of the probability density function of each parameter. We have derived the relative amount of the different dust grains in the model, the total dust mass, and the strength of the interstellar radiation field (ISRF) heating the dust at each spatial location. The relative fraction of VSGs is shown for M33 in Fig. 1 (from Relaño et al. 2018). Higher values of the relative fraction for VSGs (and lower corresponding values for the relative fraction of BGs) are located at the centre of the intense star-forming regions, consistent with the framework of the dust evolution models in Jones et al. (1994, 1996), suggesting dust grain destruction and/or fragmentation by interstellar shocks in the warm medium. We also find that the relative contribution for PAHs correlates well with the metallicity for the three galaxies of our sample. Furthermore, I will present the comparison of the relative contribution of small and large grains with recent hydrodynamical simulations [3, 4] that, for the first time, include the evolution of the grain size distribution.

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3D map of the dust distribution towards the Orion-Eridanus superbubble with Gaia DR2

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We present a study of the 3D distribution of dust towards the Orion-Eridanus superbubble, a nearby expanding structure that spans more than 1600 square degrees in the sky. We use Gaia DR2 photometry and parallax together with photometry from 2MASS and WISE to get distances and extinctions for stars towards this region.

We have developed a new method of mapping the dust distribution in 3D that considers neighbouring correlations using the Gaussian Processes, using which we derive the probability distribution of dust density at any arbitrary point towards the Orion-Eridanus region. Using the resulting maps, we examine the relation of the inferred 3D structure with the gas dynamics and the magnetic field morphology observed toward this prototypical object.

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Quantum chemistry computations as an interpretative and predictive tool for grain-induced astrochemical processes. The formamide formation case.

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Our Universe is molecularly rich and at about 200 molecular species have been detected in the ISM [1 − 3]. The usual interpretation of their formation is through a cascade of gas-phase reactions. Nevertheless, gas-phase processes alone cannot justify the abundance in the universe of even the simplest molecule, H_2 [4]. Resort to reactions occurring on surfaces of interstellar grains is mandatory to reconcile prediction with observation. The current knowledge of the chemical role played by these grains is mostly based on spectroscopic observations, helped by laboratory experiments and astrochemical models. This combination has been fruitful to obtain important information, like the composition, structural state and the chemical activity of the grains [5]. However, this approach cannot provide atomic-scale information such as the precise mechanistic steps and quantitative energetic data of the reactions that occur on their surfaces, or the exact role played by the grains in these reactions. This information gap, however, can partly be filled in by quantum chemistry computations as they are capable to simulate from an atom-based approach reactions of astrochemical interest accounting for the presence of the grains. These theoretical calculations are, therefore, a suitable tool to both interpret how a given detected species is formed, whether on a grain surface, and to predict new, alternative reaction channels, not considered in astrochemical models, which can actually contribute to the molecular cosmic reservoir. In this presentation, this dual role of the quantum chemistry calculations is shown using formamide (NH_2CHO) formation on water ice mantles as a test case [6]. On one hand, the coupling of the NH_2 and HCO radicals (the usual reaction assumed in the astrochemical models to form formamide) on a structural surface model mimicking a water ice mantle is simulated, hence providing a plausible interpretation of the astronomical observations. On the other hand, a new synthetic route based on the reaction of HCN/CN with H_2O molecule of the ice mantle is elucidated, hence predicting an additional reaction channel for the formation of formamide.

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A computational study of the reaction N(2D) + C_6H_6: Implications for the upper atmosphere of Titan

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The atmosphere of Titan is believed to be in some way reminiscent of the primordial atmosphere of Earth, being composed mainly by N_2, CH_4, simple nitriles like HCN and HCCCN, simple hydrocarbons like C_2H_6, C_2H_4 and C_2H_2, H_2 and Ar. N_2 is the prevalent species, being the 97% of the atmosphere and the second relevant constituent is CH_4 which represents an average amount of 2.7%. All the other species are present only in trace amounts, but their reactivity is very important, as suggested by the plethora of information provided by the NASA/ESA/ASI Cassini-Huygens mission. Recent investigations suggested also the presence of positive ions and negatively charged ions in Titan's ionosphere. More recent information were provided by the observations performed with the ALMA interferometer. Among the species identified by Cassini Ion Neutral Spectrometer, benzene shows a relatively important mole fraction, being 1.3×10^{-6} at 950 km. However, the low number density and low temperature conditions (94 K at the surface and up to 200 K in the upper atmosphere of Titan) do not allow reactivity among neutral closed shell molecules because of the presence of relatively high activation energy barriers. In the range of altitude where benzene is present, however, molecular N_2 is converted into atomic nitrogen or ions by energetic processes or by the interaction with EUV radiation. The dissociation of molecular N_2 induced by dissociative photoionization, galactic cosmic ray absorption, N_2^+ dissociative recombination, or dissociation induced by EUV photons produces atomic nitrogen in its electronic ground state 4S and in the first excited 2D state in similar amounts. Atomic nitrogen in its 4S ground state exhibits very low reactivity with closed shell molecules. On the contrary, atomic N in its first electronically excited 2D state shows a significant reactivity with several molecules identified in the atmosphere of Titan. Atomic N in its excited 2D state is metastable but it shows a radiative lifetime long enough to react in binary collisions with other constituents of the upper atmosphere of Titan. We have already investigated the reactions of atomic N in its excited 2D state with various hydrocarbons, like CH_4, C_2H_2, C_2H_4, C_2H_6, in laboratory experiments by the crossed molecular beam technique with mass spectrometric detection and time-of-flight analysis at different collision energies complemented by ab initio and kinetics calculations. More recently we have investigated the reaction between N(2D) and benzene which is supposed to be very relevant in the upper atmosphere of Titan, from the stratosphere up to the thermosphere where the first haze layer is located. In this contribution, we report on a theoretical characterization of the reaction involving N(2D) and benzene. The aim is to determine the chemical behavior of N(2D) with aromatic species after the previous investigation with aliphatic molecules. In particular, we wish to establish whether the aromatic ring is preserved in this reaction (as already observed in other cases) and whether the N atom is incorporated in the ring of carbon atoms, forming pyridine or its less stable isomers. Remarkably, by the analysis of the spectra recorded by the Cassini-INMS in the Open Source Ion mode the presence of a species with general formula C_5H_5N was inferred, indicating that either pyridine or one of its isomers are actually formed in the upper atmosphere of Titan starting from active forms of N. With this aim, we have performed electronic structure calculations of the stationary points along the minimum energy path. These calculations will complement crossed molecular beam experiments which are currently under way and will also be completed by kinetics calculations.

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The atomic to molecular hydrogen transition: a major step in the understanding of PDRs.

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After a long period of diffidence, the molecular complexity of the universe is now widely recognized, in great part thanks to the pioneer achievements of Xander Tielens. The basic model of Photodissociation Regions (PDRs) worked out with David Hollenbach [1] settled the frame for describing the interface between molecular gas, where stars form, and the surrounding galactic environment [2]. Indeed, only the inner molecular content of theses structures is able to cool and finally collapse to form stars.

The present review will focus on the different mechanisms involved in the atomic to molecular hydrogen transition of interstellar clouds and how they impact the physical structure of the environment. Particular emphasis on PDR models including the coupling between molecular hydrogen formation on grain surfaces; collisional excitation by H, He; ν, J dependent photodissociation and possible ν, J state dependent chemistry will be related [3, 4]. I will then show how recent Hershel observations of highly excited CO (up to J $\sim$ 15) towards the Orion Bar and NGC 7023 PDRs [5] can be accounted for in detailed isobaric PDR models. Other tracers including H_2, HD, CH^+, SH^+ are also satisfactorily explained with such models where the principal heating mechanism is provided by the impinging UV photons and subsequent collisional de-excitation cascades within rovibrationally excited H_2. The thin but extended layer of molecular emission emerging from the FUV-irradiated gas observed with the one arc second resolved observations provided by ALMA [6, 7], is readily interpreted from the generation of a high pressure zone triggered by radiative feedback. Additional energy sources such as shocks or X-rays are not necessary. A significant correlation between the gas pressure and the impinging radiation field is derived over a large range of radiation field intensities from galactic [5, 8, 9, 10, 11] and extragalactic [12] observations. These high pressures, unbalanced by the surrounding environment, seem to indicate a dynamical origin where the radiation field has a major effect. An additional goal for new PDR models[13, 14].

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Modelling of the chemistry of protoplanetary disks

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Protoplanetary disks are characterized by strong radial and vertical gradients of temperature, density and irradiation. These variations in the local physical conditions throughout the disk have a strong impact on its chemical structure. The upper layer of the disk, for instance, is largely dominated by gas-phase photo-processes (PDR layer) and mainly hosts atoms, ions and radicals while the attenuation of FUV photons in deeper regions leads to a richer gas-phase chemistry in the molecular layer. In the disk midplane, high densities and low temperatures lead to the freeze-out of almost all gas species at the surface of grains and result in the development of a complex gas-grain chemistry. Recent observations of disks with ALMA reveal that radial chemical substructures are common, likely indicative of an active gas-grain chemical coupling. Here, I present the results obtained from a new framework in which we self-consistently solve the time dependent gas-grain chemical composition of a protoplanetary disk with a structure obtained from self-consistent thermo-chemical disk modeling including dust physics. We show that chemistry of most observable species is dominated by photoprocesses; not only at the PDR surface, but also on ices close to the water condensation front where photodissociation of ices significantly affects the gas phase composition of the disk. The disk interior, where condensation of ices occurs, can be divided into three main chemical regions depending on local physical conditions: (i) a shielded, inner disk midplane where low FUV fluxes and warm dust ($T > 15K$) lead to the formation of complex organic molecules, (ii) an outer disk midplane where FUV from the ambient medium can be high, dust temperatures are low and where hydrogenation reactions dominate and, (iii) a molecular layer at $AV \sim 3\text{-}10$ and below the water condensation front where photodissociation of ices significantly affects the gas phase composition of the disk. Some of the common radicals observed in these objects (e.g., CN and C_2H) are found to exhibit two-layered vertical structure and are abundant near the CO photodissociation front and near the water ice condensation layer. Finally we show that many of the other observed gas phase species originate near the molecular layer/water ice boundary, and that their column densities are largely set by photo-processes and do not vary significantly when key disk properties such as mass and dust/gas ratio are changed.

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Future developments of IRAM instruments – or – IRAM's efforts to allow fulfilling promises

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Observations of dust and gas in interstellar space have made dramatic progress over the last 30 years. And progress will certainly not stop here. Many fundamental promises of ISM astrophysics and astrochemistry yet have to be fulfilled and IRAM's developments are focused to allow important next steps in this endeavor. Beyond the natural quest of more sensitivity and higher spatial resolution, millimeter astronomy will reach out for instrumentation which produces complete high-resolution spectral coverages and large-scale mapping. Ambitious plans for both IRAM observatories, the 30m telescope and NOEMA, are well advanced. The resulting data sets are of unseen size and complexity and will allow and demand for new approaches of data analysis and modeling.

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Prevalent complex organic molecules towards prestellar cores in the Taurus star forming region

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Examination into the origins and evolution of organic chemistry, the basis for life on Earth, in the ISM is vital to astrochemistry. It is crucial to study the formation of organic molecules in starless and gravitationally bound prestellar cores, as this primitive phase can best constrain the initial chemical conditions of star and planet formation (Herbst & van Dishoeck 2009). Prebiotic and complex organic molecules (COMs), such as methanol (CH_3OH), acetaldehyde (CH_3CHO), dimethyl ether (CH_3OCH_3), and methyl formate ($HCOOCH_3$), have all been detected in starless or gravitationally bound prestellar cores (i.e., Bacmann et al. 2012, Jiménez-Serra et al. 2016); however, the published studies have been limited to a small sample of well-studied (and in many cases, extreme) cores which may not be representative of the population of starless and prestellar cores. COMs were originally thought to form exclusively in ices on grains irradiated by UV radiation from the surrounding interstellar radiation field and forming protostar and subsequently desorbed into the gas phase. However, prestellar cores themselves do not have strong radiation fields, so alternative models using chemical energy have been developed to explain COM desorption (i.e., Vasyunin 2017). It is now believed that precursor molecules form on icy surfaces of interstellar grains and these radicals (i.e., OH, HCN, etc.,) are the ones desorbed and reactive in the gas-phase to form COMs. Understanding gas-phase abundances of COMs can tell us about the evolution history of the ices from which they are formed and frozen onto. Recently discovered, even the sugar of DNA, 2-deoxyribose, can be produced from ice mixtures consisting of H_2O and CH_3OH in the lab (Nuevo et al. 2018). Thus, to understand the origins of life, we must first understand the origin, production and distribution of prebiotic molecules. Our study targeted a large sample (31) of starless and prestellar cores, which span a wide range of dynamical and chemical evolutionary stages, within the localized L1495-B218 Taurus Star Forming Region. Regions with similar environmental conditions, such as within the Taurus Molecular Cloud, allow for robust comparisons to be made between cores. We find prevalent COMs, detecting CH_3OH in 100% of the cores and CH_3CHO in 68%. At least two transition lines of each molecule were measured, allowing us to place tight constraints on excitation temperature, column density and abundance - crucial for testing chemical desorption models. Additional mapping of methanol reveals extended structure, detected down to A_V as low as ~ 3 mag. A deep survey for COMs in the young prestellar core L1521E also detects several COMs including dimethyl ether, acetaldehyde, and vinyl cyanide. We find organics are being formed early and often along the filaments and within starless and prestellar cores in the Taurus Molecular Cloud and that these organics are abundant in the raw material hundred of thousands of years before protostars and planets form.

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The atomic envelope of molecular clouds as revealed by machine vision.

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We present the results of the analysis based on the histogram of oriented gradients (HOG), a tool developed for machine vision that we propose as a new metric for the systematic characterization of spectral line observations of atomic and molecular gas and the study of molecular cloud formation.

We characterized HOG using MHD simulations of the collision between two atomic clouds and then applied it to the observations of atomic hydrogen (HI) emission at 21 cm, from in the THOR survey, and ^{13}CO emission, from the Galactic Ring Survey, towards a portion of the Galactic plane.

We report the finding of a significant spatial correlation between the HI and ^{13}CO emission and the potential imprint of stellar feedback in the dynamics of the atomic and the molecular gas.

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Formation process of small hydrocarbons in PDRs: gas phase chemistry or fragmentation of polycyclic aromatic hydrocarbons (PAHs)?

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Hydrocarbons are ubiquitous in the ISM, yet their chemical formation paths in the ISM are not completely understood. It was found that in PDRs with low UV-flux ($\chi < 100$ in Habing units) such as the Horsehead nebula, the observed abundances of hydrocarbons were higher than those predicted by gas-phase chemical PDR models by an order of magnitude (Teyssier et al. 2004). This opened possibilities to other hydrocarbons formation mechanisms. Le Page et al. 2003 had suggested one such mechanism to be the fragmentation of PAHs. While in the PDRs with high UV-flux ($\chi \sim 10^4$ –10^5 in Habing units), such as the Orion Bar, the observed hydrocarbon abundance can be roughly explained by gas-phase chemistry (Cuadrado et al. 2015). M8, at 1.25 kpc from us and in the Sagitarius-Carina arm, has one of the highest UV-flux PDRs in our Galaxy ($\chi \sim 10^5$ in Habing units, Tiwari et al. 2018). The open young stellar cluster NGC6530, the HII region NGC6523/33, and large quantities of molecular gas are associated with M8 (Tothill et al. 2008). We performed a line survey toward Herschel 36 (Her 36), the main ionizing stellar system in M8, and an imaging survey within 1.3 x 1.3 pc around Her 36 of various transitions of C_2H and c-C_3H_2 (Tiwari et al. 2019). We aimed at obtaining their densities and abundances, to constrain the physical conditions of the gas responsible for their emission and to investigate the hydrocarbon formation mechanism. We detected 18 hyperfine structure components of C_2H (N= 1-0, 3-2, 5-4), and 5 ortho- and para- species of c-C_3H_2 (J= 2-1, 6-5, 7-6, 8-7). Using LTE techniques, we inferred the column densities of $C_2H \sim 10^{14}$ cm^{-2}and of c-$C_3H_2 \sim 10^{12}$ cm^{-2}, with C_2H being more abundant than c-C_3H_2. We found that c-C_3H_2 is a better tracer of a PDR than C_2H owing to its stronger emission from the PDR veil. We compared archival GLIMPSE 8 μm and SPIRE 250 μm continuum images with the C_2H emission maps and found that SPIRE 250 μm emission distribution follows the C_2H emission, while the spatial distribution of 8 μm PAH emission, does not follow it. Using the non-LTE RADEX modeling, we constrained the H_2 volume densities of the hydrocarbon emitting gas to 5 x 10^4 to 5 x 10^6 cm^{-3}. We also compared our observed column densities of C_2H and c-C_3H_2 with updated PDR models of Meijerink and Spaans (2005), which match the observed C_2H column densties reasonable well (by a factor ∼3) but predict higher values for c-C_3H_2 (by a factor of 10-25). This discrepancy might arise from clumpy gas structure that we do not resolve with our observations. Therefore, the column densities derived from our data should be considered to be lower limits. The spatial distribution of PAH emission does not follow the C_2H emission. This is consistent with PDR models, which do not require PAH fragmentation to explain the observed column densities of hydrocarbons in M8. This is in favour of the argument that gas-phase chemistry is able to roughly explain the abundance of small hydrocarbons in high-UV flux PDRs. We also compared our results with other high-UV flux PDRs such as the Orion Bar and different PDR models like Meudon code (Cuadrado et al. 2015). We find the observed column densities to be similar in both M8 and the Orion Bar. On the other hand, we found significant differences between the observed and the modeled column density of the c-C_3H_2 molecule. In the case of Orion it is about one order of magnitude lower than estimated from the observations. In the case of M8 the modeled column density is between one and two orders of magnitude larger than estimated from observations in line with the assumption that the determined column densities should be considered lower limits. This suggests that there might be a significant difference between the results obtained with the Meudon PDR model used by Cuadrado et al.(2015) and our PDR model based on Meijerink & Spaans (2005). We believe that the different chemical networks used in each model that lead to the formation and destruction of the c-C_3H_2 molecule, are mainly responsible for their column density predictions.

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The effect of circumstellar dust grains on the gas-phase chemistry in AGB outflows

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Asymptotic giant branch (AGB) stars contribute significant amounts of gas and dust to the interstellar medium (ISM). These stars lose their outer envelope through a stellar outflow, which creates an extended circumstellar envelope (CSE). Chemistry and dynamics are closely coupled throughout the CSE, which is especially clear in the intermediate region, where newly formed dust grains launch a dust-driven outflow.

Chemical modelling of CSEs is traditionally divided into two main groups, either modelling the non-equilibrium chemistry in the innermost region close to the star, caused by shocks due to the pulsating star, or the photon-induced chemistry in the less dense outer region. The specific chemistry of the intermediate region, where both solid-state dust grains and gas-phase molecules are present in large densities, has not previously been modelled. We have implemented dust-gas interactions and grain-surface chemical reactions in our chemical kinetics model, connecting the chemistry of the intermediate wind to that of the outer wind for the first time.

We will discuss on the different dust-gas interactions and grain-surface reactions included in our model, and their relative importance on the gas-phase chemistry. We will show results for a grid of models for both an oxygen-rich and carbon-rich chemical compositions, including the effects of different outflow densities, different types of dust grains and their corresponding temperature profiles, and different drift velocities between dust and gas.

Including dust-gas reactions affects the gas-phase molecular abundances within the intermediate and outer wind in higher density outflows. Certain parent species, present at the start of the model at 20 stellar radii, are depleted onto dust, e.g. H_2O and SiO in oxygen-rich outflows. The dust grains are therefore covered by ice mantles, especially in the case of an oxygen-rich CSE, where more than 100 monolayers are formed. Chemistry on the grain surface leads to an increased abundance of certain gas-phase species, such as hydrates. Our results show that including dust-gas reactions is crucial for the interpretation of high-resolution observations, such as the ALMA Large Program ATOMIUM, and for a complete understanding of their enrichment of the ISM.

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Astrochemistry: the next 40 years

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Xander has been well ahead of most astrochemists during the first 40 years of his career and set the research directions for several generations of researchers. What will the next 40 years bring? This talk will look into Xander's crystal ball and highlight a few areas of focus for the future, including protoplanetary disks, links with exoplanetary atmospheres and the origin of life. In addition, the importance of continued investments in laboratory astrophysics and the understanding of basic processes.

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Chemistry and isotopic ratios in intermediate redshift molecular absorbers

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The spectroscopic study of absorption lines toward bright background continuum sources provides a powerful technique to investigate the composition of the ISM in the Milky Way and in distant galaxies. These molecular absorption studies provide high sensitivity and resolution thanks to the bright background source, and opacities (and thereby column densitites) can be directly derived. However, they do require a foreground galaxy in the line of sight to a more distant continuum source, and only a handful of such systems are known. I will focus on the two best-studied systems: the absorber at z=0.68 towards the quasar B0218+357, and the absorber at z=0.89 towards the quasar PKS1830-211.

About a dozen molecular species have been detected towards B0218, and over 40 towards PKS1830, with measured isotopic ratios for C, N, O, S, Si, Cl, and Ar.

These isotopic ratios provide clues about the chemical evolution of both the individual galaxies and the cosmos, since their redshifts correspond to look-back times of about half the age of the Universe.

Recently we have used observations of the chlorine-bearing species HCl and $H2Cl^+$ in these galaxies to investigate chemical properties and Cl isotopic ratios in the absorbing sightlines. I will discuss our results of the physical properties of the absorbing gas, the nucleosynthesis history of the galaxies, and the need for a stronger interstellar radiation field in order to explain our observations.

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The dust cycle in galaxies: from stardust to planets and back

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The interstellar medium in galaxies contains a small mass fraction of solid material (dust) whose sources and sinks are a topic of ongoing studies. The composition of these solids may help to elucidate this cycle of matter and shed light on the physical and chemical conditions that govern dust formation and destruction. Vastly different environments such as the outflows of evolved stars, supernovae, the diffuse interstellar medium, the dense regions of molecular clouds and planet forming disks are imprinted in the nature of solid material and its composition. Spectroscopy from X-rays to the far-infrared, in situ studies of solar system bodies, and detailed isotopic analysis of meteoritic samples are among the powerful tools to pin down the chemical composition and lattice structure of dust in these different environments.

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The properties of silicates in the interstellar medium

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The infrared and X-ray part of the spectrum provide powerful tools to put important constraints on the properties on interstellar dust, for instance on the composition, crystallinity and size distribution of dust grains. The size distribution in particular is an important component of many dust models and there are currently many different size distribution models available. The properties of the grains in these distributions are mostly based on the properties of bulk material, although there are many small (nano size) dust grains present that may not share the properties of these materials.

Silicates are a major component of interstellar dust. Small silicate nano grains may provide insight in the formation of grains in the interstellar medium (ISM), since the observation of these small clusters may point to active grain formation in the ISM. They may also explain the absence of crystalline dust in ISM, since many atoms are near the surface of the grain, distorting the lattice structure, which may make the grains appear amorphous while they are still in their lowest energy configuration.

In order to study the small-size end of the distributions, we make use of infrared and X-ray spectra generated from calculated minimum energy structures of both cut bulk grains and the nucleation cores from Goumans and Bromley (2012) and Escatllar et al. (2019, submitted). We fit these spectra to infrared and X-ray sources in the Galaxy and present our first preliminary findings.

Furthermore we will show how we can further constrain the dust size distribution and dust composition in different environments of the Galaxy using X-ray spectroscopy techniques. Here we make use of recent laboratory dust measurements (Zeegers 2019).

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POSTER CONTRIBUTIONS

Thermal emission from the 18-cm lines of OH - a new diagnostic tool for studies of molecular gas in the Galaxy

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I will review the case for using the 18cm thermal emission lines of OH to supplement the millimeter CO lines as tracers for molecular gas in the ISM of the galaxy on the large scale. Examples will be given of applications to studies of the physical state of the ISM on parsec scales, and to the distribution and motions of molecular gas in the spiral arms of the Galaxy. Problems and prospects for the use of OH emission as a diagnostic tool will be briefly discussed.

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From protostars to protoplanetary disks: astrochemistry at work during the Class I phase

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What is the evolution of the chemical complexity during the process leading to the formation of a Sun and its planetary system? Is the chemical richness of a Solar System partially inherited from the earliest stages or do we have a chemical reset?
The first step to answer these questions is to perform a comparison between the overall astrochemical content observed in the protostellar stage and the pristine material from which our Solar System formed, contained for example in comets. On the one hand, the protostellar phase is characterized by the molecular complexity blooming due to the hot-corino phenomena. When the inner 100 au protostellar envelope are heated at temperatures larger than 100 K, dust mantles products thermally sublimate and enrich the chemical composition of the gas. On the other hand, dramatic changes in the molecular abundances are expected because of a warm gas-chemistry at work. While hot-corinos in Class 0 sources are relatively well-known, very little has been done so far to study the overall composition of more evolved Class I sources, which represent the link between the protostellar stage and the planetary system formation.

We present the first full census of the chemical content obtained in a Class I source thanks to the synergy between the IRAM-30m ASAI (Lefloch et al. 2018) and IRAM-NOEMA SOLIS (Ceccarelli et al. 2017) Large Programs. The NOEMA interferometric observations are used to study the source on a Solar System scale and they are supported by an unbiased spectral survey performed with the single-dish telescope. The results will be discussed in the context of the state-of-the-art Class I studies.The measured molecular abundances will be compared to those measured in Class 0 sources as well as in the 67P/Churyumov–Gerasimenko comet.

Future perspectives on Class I investigations will also be presented thanks to the incoming results of the ALMA Large Program FAUST (http://stars.riken.jp/faust/fausthome.html) and the ERC project “The dawn of organic chemistry” (https://doc.osug.fr/?lang=en).

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Analyzing astronomical PAH Spectra - PAHdb: an important tool of the trade

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Since the first detection of the UIR bands and the subsequent inception of the PAH model a lot of progress has been made in how infrared (IR) astronomical observations are analyzed and interpreted. The PAH community now relies on a plethora of different tools, one of them being the emergent use of databases. Perhaps the largest of these databases focused on PAHs is the NASA Ames PAH IR Spectroscopic Database (PAHdb). PAHdb hosts well over 3,000 density-functional-theory (DFT) computed and nearly 100 laboratory measured spectra. This collection of spectra contains the IR signatures of PAH molecules of different sizes, charge states, compositions and structure. In addition to housing the spectroscopic data, PAHdb also offers several software tools to help analyze and interpret the PAH features in astronomical observations. These tools incorporate the knowledge and paradigms developed over the last three-plus decades and allow the astronomical community to get the most out of their data. Access to PAHdb is organized through a web portal, located at www.astrochemistry.org/pahdb/, where visitors can peruse the contents of the spectroscopic libraries, do some rudimentary analyses, find links for downloading the spectra and software tools, and get help. Since the launch of the web portal in 2010 more than 60,000 unique visitors from 164 countries have been recorded. In the same time span PAHdb and its associated tools have been used to study a wide selection of astronomical object types, ranging from Solar System objects (e.g., Titan) to entire galaxies. Many of these studies employed novel approaches enabled by PAHdb.

One such approach is to fit the 5-12 μm interstellar PAH spectrum (not individual PAH bands) using the spectroscopic data in PAHdb. This was used to track the spectral-spatial evolution of the PAH emission bands in the Spitzer-IRS spectral maps of a number of reflection nebulae (RNe). Connecting, on a pixel-by-pixel basis, the 6.2/11.2 μm PAH band strength ratio, long known to be a qualitative tracer for the PAH ionization fraction, to the quantitative, database-determined PAH ionization parameter quantitatively calibrates this traditionally qualitative measure. Subsequently, this ties directly to parameters describing the local astrophysical environment, i.e., the temperature of the gas, the strength of the radiation field and the electron density; making the PAH features a probe of physical conditions in the emission regions.

An entirely different approach employed machine learning, which was used to cluster PAH abundance maps established from database-fits based on their structural similarity index (SSIM). This work shows that, for two fields-of-view in the reflection nebula NGC 2023, the resulting cluster maps recovered morphological features that aligned with several of the ridges clearly present in the visible maps of the region. A subsequent direct comparison with results derived using Gaussian spectral decomposition showed the two approaches augment each other.

A third example focused exclusively on the information contained within the database itself to gain insight into the molecular factors driving observed shifts in peak position of the 7.7 μm PAH emission complex. The 7.7 μm band is known to vary significantly from object-to-object in astronomical observations, but the origin of these variations remains speculative. Here the peak position of the 7.7 μm band complex in the PAHdb spectral library were analyzed as a function of PAH size, charge, composition. This application enabled by PAHdb shows that variations in PAH size can accommodate the large observed shifts in peak position, perhaps followed by PAHs with aliphatic side groups. PAH charge and composition

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In a similar, but more constrained approach, the spectral variations within a particular sub-class of PAHs are studied. The so-called ”Clar” PAHs were chosen because they represent the special sub-class of PAHs which are fully-aromatic and, therefore, particularly stable. When considering all the Clar structures possible in PAHs ranging in size from CH to CH in three charge states (+, 0, -) one reaches a total of 3,120 species. A systematic analysis of these spectra show that ”Clar” PAHs generally lack an 11.2 μm band and have blue-shifted peak positions when compared to their non-Clar counterparts in the PAHdb spectral libraries. This strongly suggests ”Clar” PAHs are not important members of the interstellar PAH population, a conclusion in line with a direct database-fit to representative astronomical observations.

Clearly, the availability of PAHdb has opened up new ways to investigate the interstellar PAH population, its response to local conditions, and the roles it plays in astronomical processes.

The use of databases in (infrared) astronomy is on the rise and with the James Webb Space Telescope on the horizon, the need for high-quality, high-fidelity data will only grow larger. Tools that are effective and up to the task of handling those data will also become more-and-more important. To that end, NASA has funded a Directed Work Package titled: Laboratory Astrophysics - ”The NASA Ames PAH IR Spectroscopic Database” that aims to extend the spectroscopic contents of PAHdb and further develop the tools necessary for astronomers to work with these spectra. PAHdb’s spectral libraries will be extended by adding the spectra of PAH species currently underrepresented: e.g., large irregular PAHs and PAHs containing nitrogen; introducing different data-types, e.g., the spectra of PAH cluster and high-resolution gas-phase spectra. The available tools are also being extended and improved, most notably underway is the work to construct a semi-empirical PAH emission model that better mimics the effects of anharmonicity on emission band peak positions, profiles and intensities.

"Density Functional Theory" study on interstellar polycyclic aromatic hydrocarbon molecules

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Interstellar Polycyclic Aromatic Hydrocarbon (PAH) molecules exist in diverse forms depending on the local physical environment of the Interstellar Medium (ISM). Formation of ionized PAHs (anions and cations) is favorable in the extreme condition of the ISM. Besides its pure form, PAHs are likely to exist in substituted forms, for example, PAHs with functional groups, dehydrogenated PAHs, protonated and deuteronated PAHs, etc [2, 3]. These PAHs may convert into alternate forms as a result of ongoing chemical processes in the ISM. Fullerene (C_{60}^{+}) has recently been detected as a crucial component of the ISM (Campbell et al., 2015; Ehrenfreund and Foing, 2015). Dehydrogenated PAHs might be an intermediary between PAHs and Fullerenes [1].

The spectral evidence of PAH molecules and its variants in the ISM are observed via the mid-infrared bands, particularly at 3.3, 6.2, 7.7, 8.6, 11.2 and 12.7 μm [6]. These bands, also known as "Aromatic Infrared Bands (AIBs)" are widely present in the ISM and arise from the vibrational relaxation of PAH molecules on absorption of background UV photons. However, the exact form of PAH molecules that are responsible for the AIBs is still ambiguous. Here, we discuss the possible form of interstellar PAH molecules as carriers for AIBs. Density Functional Theory (DFT) calculation on several classes of PAHs is employed to study its spectral characteristics in infrared. We compare our results with observations in quest of any correlation that establishes its presence in the ISM.

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Revealing the formation of cosmic fullerenes in the planetary nebula Tc 1

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In recent years, fullerenes (and in particular C_60) has been detected in a variety of astrophysical environments – from the circumstellar carbon-rich surroundings of evolved stars to interstellar reflection nebulae and young stellar objects. Understanding how these species form, evolve and respond to their environment yields important insights into astrochemistry and the characteristics of large aromatics in space, thought to be the main reservoir of organic material in space. I will present an overview of what we have learned about cosmic fullerenes from mid- and far-infrared observations (using the Spitzer Space Telescope, SOFIA/FIFI-LS and HAWC+, and Gemini/T-ReCS) of the peculiar planetary nebula Tc 1, as well as from theoretical calculations and recent laboratory experiments, and show how fullerenes have significantly changed our understanding of interstellar chemistry.

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Profile comparison of the 6 - 9μm polycyclic aromatic hydrocarbon bands in starburst-dominated sources

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Polycyclic aromatic hydrocarbons (PAHs) probably represent the main reservoir of molecular organic material in space. These molecules are of great astrochemical and astrobiological interest due to their potential to form prebiotic molecules. For instance, their simplest units with N atoms included in the aromatic rings, denominated Polycyclic Aromatic Nitrogen Heterocycles (PANHs), are involved in the production of Nucleobases, a very important issue when considering the protobiotic scenario of the PAH world. Analyses of the PAH feature profiles, especially the 6.2, 7.7 and 8.6μm mid-infrared (MIR) bands, could indicate their presence in astrophysical environments of galaxies. In this work, the bands of 126 predominantly starburst-dominated galaxies (including HII regions and Seyferts, for example), extracted from the Spitzer/IRS ATLAS project, have been fitted, and separated into the Peeters' A, B and C classes. The blueshift of the 6.2μm PAH emission band, typical of the class A objects, was attributed to PANH molecules and seems to dominate this spectral feature in starburst-dominated galaxies, suggesting a significant presence of these molecules. The 7.7μm complex is also dominated by class A objects in this sample while 8.6μm band is more representative of the class B sources. The higher correlation between 6.2 and 7.7μm bands is expected due to their same CC vibration mode. However, only 24% of the galaxies were distributed into class A objects for all three bands. Although this result does not allow us to indirectly study correlations of the PANHs emission at 6.2μm with the other bands, it highlights the complexity of PAH emission. In our sample, we can see differences in the profiles that are expected to arise, even for the same source, from astrophysical and chemical environmental conditions, including the variety of molecular species that contribute for each band emission.

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Photochemical desorption of C_2H_6 and C_3H_8 in UV-irradiated CH_4 ice

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Hydrogenation of C atoms on dust grain surfaces is expected to produce $CH_x\cdot$ and, ultimately, methane, CH_4 [2]. At the low temperatures found in the interior of dense clouds, along with H_2O, CO and CO_2, the IR band of CH_4 has been observed on icy dust grains. UV photons induce different processes in ice mantles, affecting the composition of the gas-phase abundances and the species present in the ISM.

The aim of this work is to understand the processes that occur in a pure CH_4 ice mantle submitted to UV irradiation. We studied photon-induced processes for the different photoproducts arising in the ice mantle upon UV irradiation.

Experiments were carried out in ISAC, a UHV chamber eqquiped with a cryostat and a F-type UV-lamp able to reproduce the conditions present in the ISM and the secondary UV-field. FTIR spectroscopy and QMS were used to monitor the ice mantle and the gas phase, respectively, during the formation, irradiation and warm-up of the ices.

Along the various irradiation periods, direct photodesorption of pure CH_4 was not observed (see [1]). UV photons mainly induce the formation of CH· and H· radicals. Therefore, photoproducts like H_2, C_2H_6 and C_3H_8 are formed. $^{13}CH_4$ experiments were also carried out to confirm that the results were reliable. Chemical mechanisms leading to the formation of H_2, C_2H_6 and C_3H_8 are proposed. The constant ion current generated by the photoproducts in the QMS along the irradiation steps evidenced a photochemidesorption mechanism for C_2H_6 and C_3H_8, which is, to our knowledge, the largest molecule found to photochemidesorb.

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Thermal desorption and binding energies of Formamide and Methylamine from graphite and amorphous water ice surfaces

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Complex organic molecules with more than 6 atoms are species of great relevance in prebiotic chemistry and precursors for the formation of amino acids during the course of chemical evolution leading to the origin of life in earth. These molecules are predicted to be formed in the gas phase and even by grain surface reactions.

Formamide (NH_2CHO) and methylamine (CH_3NH_2) are are the most abundantly amine - containing molecules observed in many astrophysical environments (prestellar and protostellar objects, hot corinos, massive hot cores and even in comets) $[1-3]$. The presence of these molecules in the gas phase may result from thermal desorption of interstellar ices at brightness temperatures between 100 and 200 K, where icy mantle undergo sublimation or destruction.

We present laboratory experimental results for the temperature programmed desorption of formamide and methylamine from analogues of interstellar dust grain surfaces (graphite HOPG and ASW ice). The aim of this work is to understand the interaction of these amino molecules with the water ice and compare their desorption energies [4]. Thermal desorption experiments of formamide and methylamine ices were performed with a cryogenic ultrahigh vacuum setup at surface temperatures 40-240 K, and in the sub-monolayer and monolayer regimes. Using temperature programmed desorption method and a set of independent Polanyi-Wigner equations, we provided the desorption energy distributions of these molecules from water ice surface and even from graphite substrate. We compare the diffusion and the desorption behaviours of these two molecules from water ice surfaces. Implication of the high binding energies (5050-8420 K) of these molecules with respect to that of the water ice (4930 K) is discussed.

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Infrared spectroscopy of thermally excited C_{60} fullerene: revisiting the Tc1 spectrum analysis

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C_{60} fullerene has been detected in astrophysical environments thanks to the observation by Spitzer of its characteristic mid-IR emission bands, which were first evidenced in two reflection nebulae [9] and in the Tc1 planetary nebula [3]. Detection in additional astronomical objects then followed (e.g. [5, 6, 8, 10]). In all these observational studies, the authors tried to conclude on the excitation mechanism responsible for the IR emission but faced serious difficulties to conclude. Most of the studies favored a scenario in which C60 is thermally excited in solid phase, although others preferred a gas-phase scenario in which the molecule is excited by the absorption of UV photons. To conclude on this point one has however to face the limitations in precision that are present in both astronomical data and molecular data.
To progress on this question, we have recorded the experimental IR spectrum of thermally excited C60 embedded in KBr pellets. Anharmonic factors that describe the evolution of the band positions and widths with temperature were derived. Based on the comparison with available gas-phase data [7] and our previous study on pyrene [4], we conclude on the relevance of these factors to interpret astronomical spectra. Following earlier studies [1, 3, 10], we reanalysed the Tc1 spectrum, that is the best astronomical spectrum obtained so far to study the IR emission bands of C_{60}. The positions, widths and intensities of the four fundamental bands at 7.0, 8.5, 17.4 and 18.9 μm as well as the weaker combination band at 6.5 μm (first identified in the Tc1 spectrum by[2]) were derived by subtracting at best the contamination by gas lines and other bands likely associated with large molecules other than C_{60}. The comparison of these data with experimental values allows us to conclude that the observed band characteristics are globally compatible with an average emission temperature of 600-700 K. There are still unsolved issues though, in particular the integrated intensity of the 8.5 μm, which appears to be too weak in the observations. Considering the environments in which C_{60} IR emission is observed our derived high temperatures support better a scenario in which this molecule is in gas-phase rather than in solid phase.

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Infrared spectroscopy of hot pyrene ($C_{16}H_{10}$): a combined experimental and theoretical approach

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PAHs are usually considered as the carriers of the Aromatic Infrared Bands (AIBs) observed in many astronomical objects [1]. It is now well established that the origin of the AIBs is due to IR fluorescence of large PAHs, which cool down following thermal excitation achieved by the absorption of single UV photon [6]. Modeling the IR emission spectrum of a specific PAH in a specific astronomical environment requires molecular parameters such as empirical anharmonicity factors that describe the evolution of the IR band positions and widths with temperature [8]).

We recorded variable temperature IR spectra of thermally excited pyrene ($C_{16}H_{10}$) microcrystals embedded in KBr pellets from 14-723 K [2]. For the major fundamental transitions, the evolution of the band positions, widths and integrated intensities were monitored with temperature. This large temperature window covers the crystalline and molten phases of pyrene, which enables us to get insights into the contribution of intermolecular forces to the IR spectra. Empirical anharmonicity factors were derived for both the band positions and widths. We found that only bands involving large amplitude motions of peripheral H nuclei are significantly affected by the phase change. In all other cases, the derived anharmonicity factors were found to be consistent with available gas-phase data [5]).

In parallel, we computed the anharmonic IR spectra of hot pyrene using both an ab-initio code that describes the connection between states with explicit consideration of the resonances (the new AnharmoniCaOs code of [7]) and a classical molecular dynamics (MD) approach based on the Density Functional based tight binding (DFTB) method [3] and available in the deMonNano package [4]). In this latter case, finite temperature IR spectra are derived from MD trajectories by computing the Fourier transform of the autocorrelation function of the dipole moment [9]. We will show both theoretical approaches are complementary. The first one gives a detailed picture of all sorts of couplings but is limited in the temperature one can reach (typically 600 K) due to its high computational cost. On the other hand the MD approach provides the global shape of the finite temperature IR spectra but loses the detailed spectroscopic information such as resonances, hot bands or mode identification. It can however be run at much higher temperatures (1600 K in our study), which is of relevance for astrophysical models.

In this presentation, we will show how studies on pyrene can be used as a benchmark to test the explored experimental and theoretical methods. In particular, we are interested into their capability to provide empiral anhramonicity factors in order to simulate the IR emission spectra of PAHs in astrophysical environments.

Acknowledgements

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The thermal and chemical interaction of the supernova CTB 109 with the dense interstellar medium

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Supernovae inject vast amounts of energy into the interstellar medium (ISM) shaping the chemical, thermal and dynamic evolution. Gas which is shocked by the supernova is heated to considerable temperatures and emits in the X-ray and gamma-ray bands. As such, supernovae do not interact with the ISM purely through the physical act of shocking gas but also through the production of high energy photons (and cosmic rays) which are absorbed by the surrounding ISM.

CTB 109 is an X-ray luminous supernova remnant at a distance of ∼3.2 kpc, located to the east of a giant molecular cloud. The remnant's semicircular morphology in X-ray and radio suggest the shock wave has encountered the cloud. Parts of the CO-bright cloud lie in front of the supernova remnant, making CTB 109 an excellent site for studying the influence of X-ray irradiation on the dense ISM.

We present IRAM 30m observations of the dense clumps in front of CTB 109. These observations include the (J=1-0) and (J=2-1) lines of ^{12}CO, ^{13}CO and C^{18}O, and lines from HNC, HCN, HCO$^+$ and N$_2$H$^+$. In combination with archival data in the mid- and far-infrared, X-ray and radio we characterise the morphology, dynamics, and chemical and excitation conditions of the dense heavily irradiated pre-shock gas. We find that the X-rays have caused significant heating within the clump, with dust temperatures ranging from 50 to 300 K. We see a coincident increase in the excitation temperature of ^{12}CO and ^{13}CO in the region. Moreover, we see strong spatial variations in the ^{12}CO/^{13}CO integrated intensity ratio which we interpret as chemical fractionation produced due to weaker ^{13}CO self-shielding in this highly irradiated environment. We use our new multi-band X-ray radiation module coupled to a time-dependent ISM chemistry network running on-the-fly in hydrodynamic simulations to help model the interaction and physical conditions within the clumps.

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CPIPES - Collisional + Photo Ionization Plasma Emission Software - a package for joint thermal and dynamical simulations of the interstellar medium

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CPIPES (Collision + Photoionization Plasma Emission Software) traces the evolution of the ionisation structure and emission processes of optically thin plasmas. It can be used as a standalone software or coupled to any hydrodynamical and magnetohydrodynamical software tracing the dynamical evolution of the interstellar plasma. In particular it is being used to calculate the joint thermal and dynamical evolutions of the supernova and cosmic-rays driven interstellar medium.
The physical processes included in CPIPES are electron impact ionization, inner-shell excitation auto-ionization, radiative and dielectronic recombination (followed by cascades), charge-exchange reactions (recombination and ionization), continuum (bremsstrahlung, free- bound, and two-photon) and line (permitted, semi-forbidden, and forbidden) emission. The radiative model further comprises detailed calculations of the relative populations due to electron impact excitation and de-excitation, and spontaneous emission using up to a 70-levels model. The code further includes photoionization due to an external radiation field, and inner-shell photoionization due to cascades. In addition, Auger and Coster-Kronig photo-ejection of deep shell electrons is taken into account.

CPIPES includes thermal and non-thermal distributions of electrons and protons and is used to determine the ionization structure and emission of ionized plasmas with cosmic rays.

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Interstellar complex organic molecules in the NGC 1333 IRAS 4A outflows

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Interstellar Complex Organic Molecules (iCOMs) are considered as the small bricks from which more complex and prebiotic molecules may build up. Although they have been detected in solar-type forming planetary systems since almost two decades [2], iCOMs formation is still a matter of debate.

As part of the SOLIS (Seeds Of Life in Space; [1]) Large Program with the IRAM-NOEMA (NOrthern Extended Millimeter Array) interferometer, we have obtained high angular resolution maps of several iCOMs towards the outflows emanating from the binary Class 0 protostar NGC1333 IRAS4A. This system is associated with a spectacular large-scale ($\geq$1' in size) bipolar outflow previously studied with several tracers (e.g. SiO, SO, SO_2, HCN, H_2CO: [4,5,6,8]).

The new SOLIS observations show iCOMs emission on scales of 2"-1' in these outflows, where the interaction of the violently ejected material with the surrounding quiescent gas creates shocked regions. This is the second ever outflow in the solar-mass regime, after L1157-B1 [7,3], where iCOMs have been detected and their spatial distribution imaged. We revealed a spatial segregation between different iCOMs, likely caused by an abundance time-dependence effect triggered by the release into the gas phase of precursors of the detected iCOMs. In this presentation, we will discuss how the observed chemical segregation provides new information on these outflows and puts severe constraints on the iCOMs formation routes.

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Gas-phase formation of acetaldehyde in molecular shocks

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Interstellar complex organic molecules (iCOMs: containing at least 6 atoms whose at least one is carbon: Herbst & van Dishoeck 2009, Ceccarelli et al. 2017) represent an important class of molecules detected in the Inter-Stellar Medium (ISM). They become of particularly great value when it comes to solar-type star forming regions, as they may have been inherited by the Solar System objects at its birth.

Among the detected iCOMs, acetaldehyde (CH_3CHO) is particularly interesting because it has been detected in a large variety of ISM objects, and, relevant to this contribution, in those representing important phases of early solar-type star formation: cold prestellar cores, hot corinos and protostellar molecular shocks. Therefore, is almost ubiquity demonstrates that acetaldehyde must be a relatively easy to form iCOM.

Two ways to synthesize acetaldehyde have been evoked in the literature: (1) its formation on the interstellar icy grain-surfaces via the combination of the CHO and CH_3 radicals, and (2) its formation in the gas-phase, mostly via the reaction of CH_3CH_2 and O. In this contribution, we will present theoretical predictions of the gas-phase formation of acetaldehyde and compare them with previous observations obtained towards hot corinos and protostellar molecular shocks, in order to verify whether gas-phase reactions can reproduce the observations and under which conditions.

The predictions are carried out with the upgraded version of the gas-grain GRAINOBLE code, initially developed by Taquet, Ceccarelli and Kahane in 2012. The new version of GRAINOBLE is extremely flexible and allows an easy incorporation of the several and complex processes contributing to the chemistry of interstellar objects.

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Non-thermal desorption processes: a comparison between UV, X-ray and electron induced desorption from water ice

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Non-thermal desorption processes play a key role in the exchanges between the gas phase and the icy solid phase of cold regions of the interstellar medium, where a lot of molecules are expected to freeze out on dust grains with the temperature forbidding their thermal escape. These processes have been used to explain otherwise puzzling gas phase observations of simple molecules like CO in dense cores or cold H_2O in outer parts of protoplanetary disks. They are also invoked as ways to get complex organic molecules (COMs) presumably formed on grains into the gas phase. Considerable experimental efforts have therefore been devoted to the understanding and quantification of these processes, in particular specific ones such as UV photodesorption and chemical desorption. Here we will present experimental results on non-thermal desorption processes applied to the case of water ice, the main component of ice mantles. Three different sources of non-thermal desorption have been explored: UV photons, X-ray photons and electrons. There are common points and differences between the ways these particles bring energy to the ice and induce desorption. This leads to quantitative and qualitative differences in the observed desorption and chemistry, which will be exposed here. Then, the respective possible influences of each of these processes in astrophysical media will be examined.

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Revisiting the [OH + $H_2 \rightarrow H_2O$ + H] reaction along with the ISM environment

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In spite of the permanent damage suffered from the radiation field, interstellar grains are still covered by ices mantles whose role in interstellar chemistry is well beyond any doubt. It means clearly that the destruction of the ice cover has to be counterbalanced by efficient reconstruction mechanisms. The breakdown of a water molecule leaves atomic H, O, and diatomic OH fragments that may interact between themselves and with the H_2O molecules underneath. In this contribution we focus on the [H_2 + OH] reaction that we believe decisive (Tielens & Hagen 1982) for the reconstruction of the ice mantles in view of the well-known high density of surrounding H_2. We report the results of quantum numerical simulations taking into account the involvement of the surviving icy support all along the reaction path. The calculations were performed in both cluster and solid state approaches. Although the end product is the same, namely, reconstruction of one H_2O on the subjacent ice, two different mechanisms are found, depending whether H_2 reacts with adsorbed OH or OH reacts with adsorbed H_2. In the first case, there is a reaction barrier requiring tunnel effect whereas the second case is a no-barrier reaction leading to immediate reconstruction of the ice. The prevalence of one or the other mechanism will depend strongly on the environment. The fact that two pathways are possible for the same reaction may be more general than shown here and suggests that this type of situation should be considered in current models of grain surface chemistry.

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Laboratory experiments on the carriers of the 'Class C' UIR bands

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The unidentified infrared (UIR) bands have been ubiquitously observed in various astrophysical environment. Peeters et al. (2002) classified the UIR bands observed with ISO/SWS into three classes (Class A, B and C) in terms of peak position and the profile of each band. Only two objects, AFGL2688 and IRAS 13416-6243, out of 57 objects exhibit 'Class C' UIR bands, which is predominantly characterized by the presence of broad $\sim 8.2 \mu$m feature instead of the 7.7μm and 8.6μm UIR features which are usually seen in 'Class A' and 'Class B' objects. Several more sources showing 'Class C' UIR bands are found based on Spitzer/IRS observations and Sloan et al. (2007) has reported that the Class C UIR bands are seen particularly in objects illuminated by the heating source with low effective temperatures. In addition, infrared spectra of dusty classical novae are recently found to exhibit the characteristics of the Class C UIR bands (e.g. Evans et al. 2005; Helton et al. 2011). Polycyclic aromatic hydrocarbons (PAHs) hypothesis has commonly been used to interpret the properties of the general UIR bands and, recently, mixed aromatic-aliphatic organic nanoparticles has been suggested as an alternative interpretation of the carriers of the UIR bands (Kwok & Zhang 2011). However, our knowledge on the nature of the carriers of the UIR bands, in particular those of the 'Class C' UIR bands, is still limited. We have succeeded in synthesizing laboratory organics named 'Quenched Nitrogen-included Carbonaceous Composite (QNCC)' from the plasma gas produced from nitrogen gas and hydrocarbon dust via 2.45GHz microwave discharge. We have found that infrared properties of QNCC can reproduce the characteristics of the Class C UIR bands observed around dusty classical novae. Based on the infrared microspectroscopy and X-ray Absorption Near Edge Structure (XANES) analyses of QNCC, we have found that amine structures are present in QNCC and are responsible for the broad 8μm feature of 'Class C' UIR bands. The N/C ratio of QNCC is obtained as 3-5% from the measurement with Elemental Analyzer/Isotope Ratio Mass Spectrometer (EA/IRMS).

We also recognize the similarities in the infrared and X-ray spectroscopic properties between QNCC and insoluble organic matter (IOM) in carbonaceous chondrites. We have kicked off the space exposure experiment of QNCC using International Space Station (ISS) Japanese Experiment Module 'KIBO' ExHAM. This exposure experiment aims to verify the hypothesis that organics which originates in evolved stars have delivered and contributed to primitive organics in solar system by comparing the properties of QNCC, which is a powerful candidate of the organics associated with classical novae, collected back from the space exposure experiment with those of IOM, which is an important material to investigate the nature of primitive organics in solar system. In this presentation, we will show the properties of QNCC as a powerful candidate of the carriers of the 'Class C' UIR bands and will give an introduction of our new space exposure experiment of QNCC using ISS/KIBO/ExHAM scheduled from this autumn.

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Reactivity of HCO with CH_3 and NH_2 on water ice surfaces. A comprehensive accurate quantum chemistry study

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Interstellar complex organic molecules (iCOMs) [1, 2] have a great importance for the astronomical community for several reasons, including that they can contain an important fraction of carbon in a molecular form easy to be used to synthesise more complex, even biotic molecules. Moreover, they have gained a lot of attention since the discovery of iCOMs in solar-type protostars [3, 4]. Indeed, iCOMs formed in the protostellar phase could have been inherited from the small bodies of the Solar System, e.g. carbonaceous chondrites and comets, and played a role in the origin of life on Earth [5]. Thus, understanding how iCOMs are formed and destroyed is of high importance to predict the ultimate organic complexity reached in the interstellar medium (ISM). Two paradigms are invoked in the literature. Both argue that simple molecules and atoms are hydrogenated on the interstellar grain surfaces during the cold prestellar phase. Following this first step, one paradigm assumes that iCOMs appear as a result of gas-phase chemical processes, whereas the other predicts that radical-radical reactivity on the grain surfaces is the major responsible for the observed chemical complexity. The latter is nowadays the most popular among astrochemical models, even though some basic assumption 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. Here we propose an alternative method: theoretical quantum chemistry calculations, which can provide a precious atomistic perspective from which to study such processes (e.g. [6; 7]).

In this contribution, we present our recent quantum chemical study on the surface reactivity of two radical couples: CH_3 + HCO and NH_2 + HCO. According to observational evidences, the icy mantles that cover interstellar dust grains are dominated by water [8]. We, therefore, use two cluster-like models made of 18 and 33 water molecules, respectively, to simulate the grain surface where the radical-radical reaction occurs. We then study the reactivity of the two biradical systems by means of static quantum chemical calculations to verify the formation of acetaldehyde (CH_3CHO) and formamide NH_2CHO), respectively. Besides the formation of the two iCOM, we also observe competitive processes leading back to simpler species, for example to CH_4 and CO in the first system. 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. These results indicate that the fraction of iCOMs generated in the current astrochemical models is certainly overestimated since the competitive reactions are not included.

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Coulomb explosion dissociation processes of simple organic molecules by ionizing radiations in space

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An experimental investigation on the fragmentation dynamics following the double photoionization of simple organic molecules of astrochemical interest, as propylene oxide and N-methylformamide, induced by VUV photons has been reported. Experiments used linearly polarized light in the 18-37 eV (propylene oxide) and 26-45 eV (N-methylformamide) photon energy range at the Elettra Synchrotron Facility of Trieste (Italy) [1,2]. Ion imaging and electron-ion-ion coincidence techniques are used with time-of-flight mass spectrometry [3,4]. In the case of propylene oxide, six different two-body fragmentation processes has been recorded with the formation of $CH_2^+/C_2H_4O^+$, $CH_3^+/C_2H_3O^+$, $O^+/C_3H_6^+$, $OH^+/C_3H_5^+$, $C_2H_3^+/CH_3O^+$, $C_2H_4^+/CH_2O^+$ ion pairs. The double photoionization of N-methylformamide occurs producing two main fragmentation reactions, forming $CH_3^{++}CH_2NO^+$ and $H^{++}C_2H_4NO^+$. The relative cross sections and the threshold's energy for all fragmentation channels are recorded as a function of the photon energy. In the case of the double photoionization of propylene oxide, the measure of the kinetic energy released distribution for the $CH_3^+/C_2H_3O^+$ final ions with the their angular distributions allowed the identification of a bimodal behavior indicating the possible formation of two different stable isomers of $C_2H_3O^+$: acetyl and oxiranyl cations. The obtained results are important to clarify the fragmentation dynamics of elementary processes induced by the interaction of ionizing radiations with simple organic molecules in space.

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Collisional excitation of interstellar molecules: 10 years after “The Molecular Universe”

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Alexander Tielens was coordinator of “The Molecular Universe” Research Training Network (2004-2008). This highly interdisciplinary network of European researchers was devoted to the physics and chemistry of molecules in space. Among major advances, “The Molecular Universe” initiated a number of fruitful collaborations between theoreticians and experimentalists in the field of molecular energy transfer. Inelastic collisions indeed dominate the excitation of most interstellar molecules and accurate knowledge of their rate coefficients is crucial to extract temperatures, densities and abundances from observed spectra. We will review the many efforts over the last ten years to confront theory and experiment at the state-to-state level and at very low energies, for benchmark molecules such as CO and H_2O. We will also illustrate through radiative transfer studies that a good knowledge of collision rates allows to accurately model strongly non-thermal situations such as maser action in organic molecules. Finally, the latest theoretical developments on the excitation of reactive ions (e.g. CH^+, OH^+) and the upcoming exciting perspectives in the field will be presented.

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Improving the reddening estimate for a sample of young star clusters

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The characterization of interstellar and circumstellar grains in star-forming regions provides important clues to better understand the processes that occur in the early stages of star formation. In particular the study of clusters of young stars depends strongly on the initial conditions of the original cloud in the aspects of spatial, chemical and energy distribution. Due to the interaction of starlight with dust grains, the interstellar reddening is strongly dependent of dust grains size, their distribution and cloud overdensities. Thus, in the comparison of the observational data with the theoretical models, it is necessary to correct the extinction effects. We studied a sample of 50 young star clusters located at different Galactic regions in a distance range of 100 to 3000 pc, and identified the cluster members based on Gaia DR2 data. Stellar parameters such as mass and age were obtained from the comparison of observed data with evolutionary tracks from PARSEC models. Average values for E(B-V) were estimated as part of the fitting process in the colour-magnitude diagram. We present the preliminary results of these studies and discuss the E(B-V) for the sample. Thanks to the accuracy of the Gaia data, it was possible to better determine the values of the distances, indicating that many values of E(B-V) found in the literature could be better determined, with the consequent improvement of clusters age.

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Discovery of a new mechanism of dust destruction in strong radiation fields

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Massive stars, supernovae, and kilonovae are among the most luminous radiation sources in the universe. Observations usually show near- to mid-infrared (NIR-MIR, 1-5$\sim$micron) emission excess from H II regions around young massive star clusters (YMSCs) and anomalous dust extinction and polarization towards Type Ia supernova (SNe Ia). The popular explanation for such NIR-MIR excess and unusual dust properties is the predominance of small grains (size a<0.05micron) relative to large grains (a>0.1micron) in the local environment of these strong radiation sources. The question of why small grains are predominant in these environments remains a mystery. Here we report a new mechanism of dust destruction based on centrifugal stress within extremely fast rotating grains spun-up by radiative torques, namely the RAdiative Torque Disruption (RATD) mechanism, which can resolve this question. We find that RATD can destroy large grains located within a distance of $\sim$ 1 pc from a massive star of luminosity L$\sim$ 10^4L$_\odot$ and a supernova. This increases the abundance of small grains relative to large grains and successfully reproduces the observed NIR-MIR excess and anomalous dust extinction/polarization. We show that small grains produced by RATD can also explain the steep far-UV rise in extinction curves toward starburst and high redshift galaxies, as well as the decrease of the escape fraction of Ly-alpha photons observed from HII regions surrounding YMSCs.

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Discovery of a new mechanism to release complex molecules from icy grain mantles around young stellar objects

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Complex organic molecules (COMs) are increasingly observed in the environs of young stellar objects (YSOs), including hot cores/corinos around high-mass/low-mass protostars and protoplanetary disks. It is widely believed that COMs are first formed in the ice mantle of dust grains and subsequently released to the gas by thermal sublimation at high temperatures ($T>100$ K) in strong stellar radiation fields. In this paper, we report a new mechanism that can desorb COMs from icy grain mantles at low temperatures ($T<100$K), which is termed rotational desorption. The rotational desorption process of COMs comprises two stages: (1) ice mantles on suprathermally rotating grains spun-up by radiative torques (RATs) are first disrupted into small fragments by centrifugal stress, and (2) COMs and water ice then evaporate rapidly from the tiny fragments (i.e., radius $a <$1nm) due to thermal spikes or enhanced thermal sublimation due to increased grain temperature for larger fragments ($a>1$ nm). We discuss the implications of rotational desorption for releasing COMs and water ice in the inner region of protostellar envelopes (hot cores and corinos), photodissociation regions, and protoplanetary disks (PPDs). Finally, we find that large aggregates ($a\sim$ 1-100 micron) exposed to strong stellar radiations can be disrupted into individual icy grains via RAdiative Torque Disruption (RATD) mechanism, which is followed by rotational desorption of ice mantles and evaporation of COMs. In the RATD picture, we expect some correlation between the enhancement of COMs and the depletion of large dust grains in not very dense regions of YSOs.

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Extinction mapping of pre-stellar cores

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The James Webb Space Telescope presents the opportunity for substantial progress in the study of the evolution of ice mantles on dust particles in molecular cores due to its unprecedented sensitivity at thermal infrared wavelengths. Our NIRCam guaranteed time project # 1187 "Extinction Mapping of Pre-stellar Cores" will use slitless grism spectroscopy with NIRCam to obtain R>1000 spectra of background stars behind molecular cores over the wavelength range from 2.6 - 5.0 micro-meters. These will cover the prominent H_2O, CH_3OH, CO_2, and CO ice features and the spectral resolution will allow a detailed study of absorption band profiles, in particular the long wing of the H_2O feature and the CH_3OH feature.

We have selected three molecular cores in different evolutionary stages: B68, a quiescent molecular core, L694-2, a collapsing core, and B335, a protostellar core. All three cores are situated against a dense field of background stars in the inner Galaxy, maximizing the number of lines of sight through the cores and thereby the effective spatial resolution of the resulting extinction maps.

In order to cover the full spectral range of interest, we will use 6 different wide and medium filters in conjunction with the NIRCam grism. The individual spectra will be short, and spectrum overlap is not a prohibitive problem. We will obtain a few hundred spectra per target core, an order-of-magnitude improvement over existing studies, allowing us to map the spatial distribution of the ice features with a spatial resolution of about 10 arcsec. Our data will also contain regions of feature-free continuum extinction, which will allow to distinguish the effects of continuum extinction from ice feature absorption. These data will be the basis for future detailed comparisons with theoretical and laboratory models of ice mantle formation and grain surface chemistry. We will also obtain very deep continuum images with parallel observations with the short-wave channel of NIRCam for detailed mapping of the continuum extinction and studies of the core-shine in the target molecular cores.

This talk will discuss the choice of JWST instrument for this program: NIRCam vs. NIRSpec, and the detailed implementation of this program.

Ground-based preparatory work for this project will be presented separately by L. Chu et al. at this conference.

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NGC 1977 an edge-on PDR

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Orion A has always been a template region for PDR studies. Detailed investigations of the major HII regions M42, M43 and NGC 1977 showed that the associated OB clusters are responsible for their excitation. Most of the observations in the optical, IR, and submm focused on the famous M42 region and on the Orion Bar. However, the individual PDR layers in the Orion Bar are very narrow, separated by only ∼20" and thus are difficult to resolve. NGC 1977, which is located in the northern part of Orion A, shows a similar stratified, edge-on PDR structure in the Herschel temperature and density maps. But in contrast to the Orion Bar the layering extends over a few arcmins. The PDR was observed in 2017 in the [CII] 158 μm line as part of the Orion A large mapping program (PI A. Tielens) with upGREAT onboard SOFIA. An analysis of the [^{13}CII] hyperfine transition lines showed that the observed [CII] emission is strongly affected by self-absorption. The determined optical depth varies in this region between $\sim$ 3-7. This contradicts the general picture of an optically thin [CII] layer (optical depth $\sim$ 1) predicted by many PDR models. Subsequently, we observed NGC 1977 in [CI], ^{12}CO and ^{13}CO using APEX (PI Kabanovic). Again, we observe a layered PDR structure similar to the one in the Orion Bar with the [CI] layer sandwiched in between [CII] and CO. In a second step we estimate the physical parameters of the gas through a two-layer multicomponent fit to the line profile. As a result, we find that the bright rim in NGC 1977 is optically thick in [CII] with high column densities. This can be explained by a clumpy structure of the emitting gas, confirming that most of the line intensities can only be explained by PDR models involving a clumpy cloud structure such as the KOSMA-tau PDR model. However, the origin of the cold foreground gas remains open.

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CO-dark H_2 gas is not dark anymore

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The hydrogen fluoride (HF) molecule is seen in absorption in the interstellar medium (ISM) along many lines of sight. It is surprisingly observed in emission toward the Orion Bar, which is an interface between the ionized region around the Orion Trapezium stars and the Orion Molecular Cloud. We aim to understand the origin of HF emission in the Orion Bar by comparing its spatial distribution with other tracers. We examine three mechanisms to explain the HF emission: thermal excitation, radiative dust pumping, and chemical pumping. We use a Herschel/HIFI strip map of the HF J= 1-0 line, covering 0.5' by 1.5' oriented perpendicular to the Orion Bar. We use the RADEX non-local thermodynamic equilibrium (non-LTE) code to construct the HF column density map. We use the Meudon PDR code to explain the morphology of HF. The bulk of the HF emission at 10 km/s emerges from the CO-dark molecular gas that separates the ionization front from the molecular gas deeper in the Orion Bar. The excitation of HF is caused mainly by collisions with H_2 at a density of 10^5 cm^{-3} together with a small contribution of electrons in the interclump gas of the Orion Bar. Infrared pumping and chemical pumping are not important. We conclude that the HF J= 1-0 line traces CO-dark molecular gas. Similar, bright photodissociation regions associated with massive star formation may be responsible for the HF emission observed toward active galactic nuclei.

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Characterising the PAH emission in the Orion bar using Spitzer spectroscopy

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We present 5 - 14 micron spectra at two different slit positions across the Orion Bar obtained using the SL mode of the Infrared Spectrograph onboard the Spitzer Space Telescope. These spectra allow us to measure the prominent Polycyclic Aromatic Hydrocarbon (PAH) emission features at 6.2, 7.7, 8.6, 11.2, and 12.7 micron along with atomic recombination lines from hydrogen, argon, sulfur and neon. We complement these spectra with previous observations of the Orion Bar obtained with the Stratospheric Observatory for Infrared Astronomy (SOFIA) allowing for a direct comparison of the 3.3 micron PAH emission feature with the other aforementioned PAH bands. We investigate how these emission features are correlated and vary in terms of relative intensities with distance from the primary illuminating source in the nebula and with respect to the edge-on photodissociation region (PDR) front defined by the H_2 peak. We find that all the major PAH bands peak between the ionization front, defined as the transition zone between the HI/HII and the PDR front while variations between these bands become more pronounced moving away from this peak. Correlations are found between the 6.2, 7.7, 8.6 micron bands and between the 3.3 and 11.2 micron at the PDR front but generally fails to hold closer to the illuminating source and beyond the Bar. We investigate the relative behaviour of the PAH bands and relate to the intrinsic PAH properties such as size and charge.

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Survivability of PAHs: laboratory investigations on statistical dissociation processes

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Dehydrogenation and loss of acetylene are the two most important and energetically most favorable channels for internally heated PAHs. These decay channels are studied for various types of excitation processes to understand and evaluate their time constants. One aspect of the stability is attributed to electronic structure and collective excitation of these molecule when subjected to higher energy loss. And an experimental setup is developed to investigate the structural attributes of PAH molecule to survive low energy impact induced by mid band UV photon absorption.

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Deuterated complex organic molecules in low-mass Class 0 protostar regions: new results from ALMA-PILS

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The earliest stages of the low-mass star formation are characterised by a great molecular diversity in various environments. In particular, complex organic molecules (COMs) are very abundant in the deepest region of the protostellar envelope, where the dust and the gas are warmed up by the forming protostar. Despite their high abundances, many questions remain concerning the formation of such molecular species, especially whether they are formed on ice surfaces and then released during the warm-up phase or they react directly in the warm gas phase. In order to address these questions, the detection of less abundant isotopologues is crucial. The ALMA interferometer is particularly suited to carry out this kind of observations, because of the sensitivity coupled to the angular resolutions reached. Recently, the Protostar Interferometric Line Survey (PILS; [7]) has proven the ability of ALMA in detecting very faint species towards the class 0 binary protostar IRAS 16293-2422, such as CH_3Cl [6], CH_3CNO [9, 12], CH_3NC [1], NH_2CN [4] and HONO [5] for the first time in the ISM. Larger carbon chain COMs have also been detected, as for example methoxymethanol and ethyl methyl ether [11]. In addition, many singly-deuterated isotopologues were found in the observations, such as deuterated ethanol, acetaldehyde, ketene and acid formic [8] and deuterated formamide [4] and even doubly-deuterated methyl cyanide (CHD_2CN; [2]), formaldehyde (D_2CO; [15]) and methyl formate (CHD_2OCHO; [11]), for the first time in the interstellar medium. The D/H ratio of most of the detected species measured towards both components of the binary system was found to be of the order of 10^{-2}. The D/H ratio of deuterated isotopologues for the same species are very close (i.e. the abundance ratio of CH_2DOH/CH_3OH and CH_3OD/CH_3OH is close to the stoichiometric ratio of 3:1). In addition, N-bearing species have in general a lower D/H ratio than O-bearing species, however, no strong correlation has been found between the D/H ratio and the chemical group, for example between $-CH_3$ and -CHO groups. Interestingly, the D/H ratio of doubly-deuterated species is much more enhanced than the singly-deuterated conformer. In order to interpret this D/H ratio behaviour, two chemical scenarios are suggested. The first relies on experiments of deuterium substitution (H-D substitution) in ethanol and dimethyl ether on low-temperature ice surfaces [13, 14]. The author noticed that the D/H ratio of $-CH_3$ group in these two species was increased when gaseous HD molecules interacted with the ice surface. Similar chemical processes could be involved in the D/H ratio enhancement of other $-CH_3$ bearing molecules, such as in our case methyl formate. However, the H-D substitution was not observed for -CHO and -OH groups. In addition, the D/H ratio of CH_3OCDO and CH_2DOCHO are similar towards both IRAS16293A and B. The second scenario suggests that the deuteration enhancement of methyl formate is inherited from their precursors, which are HCO and CH_3O radicals, formed in turn by photodissociation of H_2CO and CH_3OH. The D/H ratio inheritance is also supported by the higher D/H ratio of D_2CO compared to the D/H ratio of HDCO. However, The measurement of D/H ratio of CHD_2OH could not be derived due to the lack of available spectroscopic data. The D/H ratio enhancement of doubly-deuterated COMs could be characteristic of IRAS16293 binary system. Therefore, more observations are needed towards other star formation environments to understand the underlying processes that increase the D/H ratio with the degree of deuteration of COMs.

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An experimental study of the pyridine (C_5H_5N) + O atom reaction: gas-phase destruction routes of a long searched molecule in extra-terrestrial environments.

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Pyridine (C_5H_5N) is a heterocyclic aromatic molecule of great interest in the astrochemical and astrobiological community being a key precursor of biomolecules which are essential for life as-we-know-it to emerge. For instance, the functionalization of pyridine with a carboxylic group (-COOH) leads to niacin, also known as vitamin B3, and C_5H_5N can also be regarded as a precursor of pyrimidine ($C_4H_4N_2$), molecular skeleton of important nucleic acids (cytosine, uracil and thymine). These species, among many other amino acids, have been found in carbonaceous meteorites [1,2] bringing an important evidence in support of the theory for "exogenous" delivery of life on Earth. However, detection of C_5H_5N in the interstellar medium [3] and in the extra-terrestrial atmospheres, such as on Titan, remains elusive still. Nonetheless, the Ion Neutral Mass Spectrometer onboard the Cassini spacecraft measured a mass-to-charge ratio that is compatible with the detection of protonated pyridine [4]. Indeed, laboratory investigations can guide and explain astronomical observations by studying the reactivity and the survival of C_5H_5N (and of other N-containing aromatic molecules as well) in Space. Unfortunately, only a limited number of laboratory experiments of this kind is available in the literature [5-10].
Within this context, we performed crossed molecular beams (CMB) reactive scattering experiments coupled with time-of- flight (TOF) mass spectrometry detection to investigate the reactivity of O atoms with C_5H_5N in single-collision conditions. Center-of-mass product angular and translational energy distributions are derived from product angular and TOF distributions in the laboratory frame. Preliminary analysis reveals that the reaction C_5H_5N + O(3P, 1D) leads to 1) the addition of the O atom to the aromatic ring via H abstraction (C_5H_4NO + H), and 2) to ring contraction via CO elimination (C_4H_5N + CO). Implications in O-rich space environments are briefly discussed.

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Theoretical study of the reaction mechanism for the formation of naphthalene by HAVA mechanism

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Studies by Parker [1] and Zhao [2] have demonstrated that HAVA mechanism presents a barrierless reaction route for the formation of PAHs [3]in low temperature environments such as cold molecular clouds. These studies have confirmed their findings via computational works, unveiling the thermochemistry of the reactions involved. Nevertheless, the mechanism of the reaction has yet to be elucidated.

In this work we present a Density Functional Theory (DFT) [8] study of the reaction between vinylacetylene and benzene to form naphthalene. Fifteen functionals were analyzed and compared based on energetic parameters. For each functional, data was obtained with different basis sets and compared to data obtained for each optimized geometry through single point calculations using CCSD(T). In order to select the best combination for the system under study, a comparison parameter was built in such a way to include the effects on both dissociation and reaction energies. Having chosen a functional and basis set, the energy profile for the reaction via HAVA mechanism of benzene and vinylacetylene was obtained. For each kinetic step of the reaction, the reaction force profile [9] is partitioned and analyzed in order to reveal the contribution of the different works to the activation energy barriers [10]. This analysis provides a characterization of the nature of these barriers, exposing the influence that electronical and structural changes may have in each step of the reaction and hence renders important information on the reaction mechanism.

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Photochemistry vs. radiation chemistry of cosmic ice analogs

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

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The effect of new H_2-H collisional rate coefficients on H_2 excitation in C-type shocks

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We consider the collisional excitation of ro-vibrational levels of H_2 molecule and the para-to-ortho H_2 conversion in C-type shocks propagating in dense molecular clouds. New data on collisional rate coefficients for the (de-)excitation of H_2 molecule in collisions with H atoms and new H_2 dissociation rates are used. Lique (2015) reported nearly exact quantum time-independent calculations of rate coefficients for the collisional (de-)excitation of H_2 by H atoms. These new data are based on a highly accurate H_3 global potential energy surface, and the reactive hydrogen exchange channels are taken into account rigorously. Bossion et al. (2018) reported quasi-classical trajectory calculations of rate coefficients for the collisional (de-)excitation of H_2 by H atoms (including the three-body collisional dissociation) for almost all ro-vibrational energy levels of the ground electronic state. In the present paper, the new rate coefficients of H_2-H collisions are incorporated into a C-type shock model propagating in a dense molecular cloud published by Nesterenok (2018). We re-examine (i) the excitation of ro-vibrational levels of H_2 molecule, (ii) the para-to-ortho-H_2 conversion, and (iii) H_2 dissociation by H_2-H collisions. The effect of the elevated levels of cosmic ray ionization rate on these processes is considered.
The simulations of C-type shock consist of two steps: modelling of the chemical evolution of a static molecular cloud and shock simulations. The rate of para-to-ortho-H_2 conversion in the shock is determined by the abundance of atomic hydrogen. Usually, the gas-phase production of water from atomic oxygen is considered as the main source of H atoms in warm gas at low and moderate shock speeds (e.g. Neufeld et al. 2006). Most of the oxygen is locked up in H_2O on icy mantles of dust grains in our model, and this channel is not so effective in H atom production as considered in previous works. The gas-phase chemical reactions (production of water, methane, ammonia) have noticeable effect on the abundance of atomic hydrogen in the shock only at low cosmic ray ionization rates. At cosmic ray ionization rates of the order of $10^{-16} \sim s^{-1}$ and higher, and at moderate shock speeds, the H/H_2 ratio in the shock is mainly determined by the cosmic ray ionization rate. The H_2 ortho-to-para ratio (OPR) and column densities of ro-vibrationally excited H_2 levels in the shock are found to depend strongly on the cosmic ray ionization rate. The data reported by Lique (2015) predict lower by a factor 1-3 para-to-ortho-H_2 transfer rates than the data by Wrathmall et al. (2007) with the inclusion of reactive channels as in Le Bourlot et al. (1999). The initial part of the shock, where the gas temperature is relatively high but H_2 OPR has not enough time to reach the high-temperature limit, makes a non-negligible contribution to the total H_2 emission. The H_2 OPR integrated over the shock length is lower than high-temperature equilibrium value for most of the shock models at cosmic ray ionization rates less than $10^{-15} \sim s^{-1}$. It is valid for energy levels of both the ground and vibrationally excited states of H_2 molecule.

We discuss the applicability of the presented results in interpretation of observations of H_2 excitation in supernova remnants.

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A new model for molecular hydrogen in galaxy simulations

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We introduce non-equilibrium molecular hydrogen chemistry into the radiation hydrodynamics code Ramses-RT. This is an adaptive mesh refinement grid code with the hydrodynamics coupled to moment-based radiative transfer. The H_2 physics that we introduce are formation on dust grains, gas phase formation, formation by three-body collisions, collisional destruction, photodissociation, photoionization, cosmic ray ionization, and self-shielding. In particular, we implement the first model for H_2 selfshielding that is tied locally to moment-based radiative transfer by enhancing photodestruction. This self-shielding from Lyman-Werner line overlap is critical to H_2 formation and gas cooling. We use this recipe for the multi-scale analysis of H_2 in a Milky Way-like simulated galaxy. Our census covers the gas content of the entire disc, to radial profiles and the Kennicutt-Schmidt relation, to a study of its molecular clouds, and finally down to a cell-by-cell analysis of the gas phases. Apart our pieces of galactic analysis are disparate, but assembled they provide a cohesive portrait of H_2 in the interstellar medium. H_2 chemistry on the atomic scale is sufficient to generate its dynamics throughout an entire galaxy. A significant fraction of the H_2 gas is in low-density regions mixed with atomic hydrogen and would therefore be difficult to observe.

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Chemical differentiation in the Protostellar system CepE-mm

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It is now well established that Complex organic molecules (COMs) and carbon-chains can be detected in the early stages of solar-like protostars. They reveal two different chemical pathways in these regions: hot corinos, rich in COMs, and WCCC sources, rich in carbon-chains. We report here a systematic study of the isolated IM Class 0 protostar CepE-mm carried out with the IRAM 30m antenna and the NOrthern Extended Millimeter Array (NOEMA) interferometer.

At large-scale, the CepE-mm envelope displays the signatures of both chemical classes, with hints of a spatial segregation between COMs and C-chains. We analyze the effects of the chemistry associated with IM protostars on COMs and carbon-chains molecular abundances. We compare its composition with typical low- and high-mass protostellar sources.

At small-scale, NOEMA unveils CepE-mm as a protostellar binary and unveils the spatial segregation between the COMs and C-Chain emissions. A strong chemical differentiation is observed between the members of the binary, with a rich molecular content towards the stronger continuum source. The fainter continuum source seems to be devoid of any molecular emission, although its drives a powerful molecular jet. We will discuss the properties of this chemical differentiation.

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The PDR structure around compact HII regions in the S235 complex

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While extended HII regions often have complicated structures, embedded compact HII regions might have geometries that are closer to spherical. We tried to model the expansion of the compact HII regions S235A and S235C in terms of a spherically symmetric setup or setups composed of two hemi-spheres representing the density gradient across the sources. At an expansion velocity around 2km/s, the PDR models reproduce the observed line profiles of [CII] and molecular lines but recent follow-up observations of [13CII] and [OI] with upGREAT onboard SOFIA show that the fine structure lines are heavily self-absorbed, having large optical depths. We deduce C^+ columns that correspond to visual optical depths of 30-40 magnitudes in contrast to our own PDR model and many other existing ones. In several lines of sight C^+ is the dominant C-bearing species. In spite of the apparent simplicity of the sources, an explanation of the large columns of warm and dense PDR material cannot be provided by one-dimensional models but requires a highly inhomogeneous structure, composed e.g. from evaporating globules around the HII regions that are best modelled through a clumpy PDR model. Eventually the density distribution around the sources is highly inhomogeneous. Gas components neither visible in [CII] nor in low-J CO may contribute to the total column in several points across the sources.

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The expanding Orion nebula - a C^+ square-degree map in the Orion A molecular cloud

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We have surveyed a ∼1 square degree area centered on the Orion Nebula in the [CII] 1.9 THz line using the heterodyne upGREAT instrument on the Stratospheric Observatory For Infrared Astronomy, resulting in some 2 million spectra at a spatial resolution of $16''$. This is the first large-scale velocity-resolved map of the [CII] fine-structure emission of this region. These data allow us to study the detailed kinematics of the region and we detect multiple bubbles in this region. Here, we will focus on the large bubble associated with the Orion Veil, blown by the stellar wind from the central star, θ^1 Orionis C. We derive the kinetics of the flow and compare our findings with models of wind-blown bubbles. Moreover, we investigate the morphology of the [CII]-emitting gas by comparison with other traces of UV-illuminated gas and dust.

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A key parameter to astrochemistry: the adsorption energy

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Actually a top priority of astrochemistry is to investigate the role of interstellar surfaces. Gas phase chemistry alone cannot account for the abundances of complex molecules (COM) observed in the ISM; solid-gas reactions and chemical processes have to be taken into account, which means implication of adsorbed partners. Moreover, the mere release of molecules from grains depends strongly of the environment, which has a direct influence on the measured molecular abundances in the gas phase. These facts make adsorption energies a key factor for the observation of molecules and their abundances in the gas phase. In spite of the strong demand from modelers, too little quantitative data are available. Grain models have been proposed such as ices, refractory minerals and carbonaceous dust particles. Though the last two cases, often qualified by the generic name of "bare" surfaces, only begin to be taken into consideration, water ices which constitute a major part of the condensed matter of the ISM are preferentially aimed at. Most of these ices are believed to be in amorphous phase, though crystalline ices have also been detected in warmer regions. The adsorption energies can be determined experimentally by TPD techniques [1,2,3], theoretically by quantum chemistry computations [3,4,5]. In both cases, the procedures are sensitive, not at all straightforward.
We propose here a review of the difficulties and possibilities for the theoretical determination of such energies, using solid state technics. When available, we compare our results to experimental ones.

- The difficulty of representing weak interactions and the choice of adapted methodology will be approached.
- In a periodic representation there is no limitation to the surface size that is treated as the frontier of a solid of infinite dimensions. However, contrary to what is generally thought, not only regular crystalline representation is possible, and we will show that other types of surfaces can be modeled.
- The problem of the multiplicity of possible adsorption sites on the surface will also be considered.

Such methods can give reliable adsorption energies though they have a real cost in human and computer time. Some demonstrative examples of astrochemical implications will be presented.

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Characterizing IC59 and IC 63 through IR observations

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The mid-IR spectra of photodissociation regions (PDRs) are dominated by the well-known emission features at 3.3, 6.2, 7.7, 11.3, and 12.7 micron, generally attributed to polycyclic aromatic hydrocarbon molecules (PAHs). PAHs drive much of the physics and the chemistry in these PDRs, e.g. by heating the gas and as a catalyst in the formation of molecular hydrogen on their surfaces. Thus, PAHs and PDRs are intimately connected, and a complete knowledge of PDRs requires a good understanding of the properties of the PAH population and vice-versa, a complete knowledge of the PAH population requires a good understanding of the local physical conditions.

Here we present a general description of two PDRs, IC63 and IC59, from an observational standpoint in order to study the physical conditions at the UV-illuminated surfaces of these objects and their PAH properties. IC63 and IC59 are a pair of cometary-shaped nebulae in the vicinity of the star gamma Cas (also known as Tsih, "the Whip"). Both nebulae have very different optical appearances, despite the fact that both objects lie at similar projected distances from the star: IC63 shows bright rims and filaments, while IC59 looks more homogeneous and fainter.

We use the available data on both nebulae taken with Spitzer, Herschel and SOFIA to study the infrared emission at the tip of both clouds, and derive the intensity of the UV radiation field, the density and the gas temperature. We find that the PAH emission is very similar at the tip of both nebulae. Even though it varies in intensity between the two, the derived PAH band ratios are remarkably similar. These ratios are similar to those found in the more shielded regions of other nebulae such as NGC7023 and NGC2023. Regarding the physical conditions, we obtain that while in IC63 the intensity of the UV field, G_0, is a factor of $\sim$10 higher than in IC59, the density n at the tip of IC59 is lower than in IC63 by a similar factor. For both objects we derive G_0 values significantly lower than what previous works have so far assumed. Comparison with other reflection nebulae PDRs and known correlations support our claim that both IC63 and IC59 are low-UV irradiated environments. We conclude that the tips of IC63 and IC59 are about 3 and 5 times farther away from the star than their respective projected distances. The similarity of the mid-infrared emission between the two nebulae is consistent not only with both objects being overdensities within the same region around γ Cas, but it is also consistent with the similar G_0/n ratio and ionization parameters, which altogether rule the evolution of the hydrogenation and ionization level of the emitting population of PAHs. Finally, regarding the kinematics of the material in IC59, we find evidence of photoevaporation due to the incident radiation from γ Cas.

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The JWST-ERS program ID 1288: radiative feedback from massive stars

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Massive stars disrupt their natal molecular cloud material by dissociating molecules, ionizing atoms and molecules, and heating the gas and dust. These processes drive the evolution of interstellar matter in our Galaxy and throughout the Universe from the era of vigorous star formation at redshifts of 1-3, to the present day. Much of this interaction occurs in Photo-Dissociation Regions (PDRs) where far-ultraviolet photons of these stars create a largely neutral, but warm region of gas and dust. PDR emission dominates the IR spectra of star-forming galaxies and also provides a unique tool to study in detail the physical and chemical processes that are relevant for inter- and circum- stellar media including diffuse clouds, molecular cloud and protoplanetary disk surfaces, globules, planetary nebulae, and starburst galaxies. We propose to provide template datasets designed to identify key PDR characteristics in the full 1-28 μm JWST spectra in order to guide the preparation of Cycle 2 proposals on star-forming regions in our Galaxy and beyond. We plan to obtain the first spatially resolved, high spectral resolution IR observations of a PDR using NIRCam, NIRSpec and MIRI. We will observe a nearby PDR with well- defined UV illumination in a typical massive star-forming region. JWST observations will, for the first time, spatially resolve and perform a tomography of the PDR, revealing the individual IR spectral signatures from the key zones and sub-regions within the ionized gas, the PDR and the molecular cloud. These data will test widely used theoretical models and extend them into the JWST era. We will assist the community interested in JWST observations of PDRs through several science-enabling products (maps of spectral features, template spectra, calibration of narrow/broad band filters in gas lines and PAH bands, data-interpretation tools e.g. to infer gas physical conditions or PAH and dust characteristics). This project is supported by a large international team of one hundred scientist collaborators.

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The PDR toolbox: past and future

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Twenty years ago, we launched the Photo Dissociation Region Toolbox (PDRT) as part of our Web Infrared ToolShed (WITS). In this poster, we review where PDRT has been and where it is going. PDRT, based on the PDR models of Wolfire et al.(1990) and Kaufman et al. (1999, 2006), is designed to help astronomers determine the physical parameters of photodissociation regions from observations. Users enter the flux and errors of their lines or continuum and PDRT does a fit to find the best interstellar FUV radiation field $\mathbf{G}_0$ and hydrogen number density **n.** Despite lack of continuous funding we have kept PDRT going because we view it as an important science-enabling tool for the community (as evidenced by the many papers published using PDRT products). Over the years, we increased the number of spectral lines covered to keep up with new telescopes and missions, added low metallicity models, and shepherded it through multiple computer replacements and operating system upgrades.

Recently we were awarded funding to make significant improvements both in the models PDRT presents and the underlying software infrastructure. Our PDR code has already been upgraded to provide more accurate physics and chemistry, including molecular freeze-out, updated collision and chemical rates, and new chemical pathways, in particular for oxygen chemistry.

We will deploy updated models that include all these improvements and allow future updates to be easily implemented so that users always get the best current model. We will also rewrite the underlying web code from scratch using modern design principles and give users more control through Python notebooks.

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On non-spherical dust grains growing in ISM

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The interstellar dust grains are known to form and grow in the vicinities of evolved stars: red (super)giants and supernova. The growth of the dust grains also occurs in molecular clouds. In this paper we present our studies related to non-spherical particles that are the results of such growth. The solid particles forming in circumstellar shells are believed to be as large as about 0.5 micron. This dust can be diagnosed from observed scattered radiation that shows a high degree of polarization [1]. The interpretation of the polarized scattered radiation has been made just with compact spherical particles. However, it is well known that, when the particle size is larger than the wavelength of the incident radiation, the scattering properties of spheres and those of particles of other less perfect shapes can differ significantly [2]. We find that the interpretation of available polarimetric observations of light scattering from clumps in the CS shells using any non-spherical particles meets serious problems.

Accretion and coagulation significantly increase the size of dust grains inside molecular clouds. It is manifested in different ways [3]. We made multiband polarimetric observation of stars seen through outer layers of the typical globule Barnard 5 and found large values of the maximum polarization position (λmax $\sim$ 0.6-0.8 micron) correlating with extinction Av in the globule. This indicates that in outer regions (Av $<$ 3 mag) where the icy mantles do not form the mean size of dust particles is nevertheless significantly larger than in the diffuse ISM surrounding the globule. So, either grains in outer layers can grow as well or there is some dust exchange between the outer and inner layers of globules.

The growth of dust grains in molecular clouds should lead to formation of aggregated particles. These non-spherical particles should be aligned and produce to observable polarized thermal emission. So far, such emission has been modelled with homogeneous spheroids [4, 5]. We have made the first calculations of the wavelength dependence of polarization degree of thermal emission from aligned aggregated particles of different kinds. We have also reanalyzed the recent observational work of [6] which claims that a region of diffuse ISM showing a high degree of sub-mm polarization measured at Planck is characterized by unusually high ratio of the degree of visual polarization to extinction. We show that it may an artefact.

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High-resolution mid-infrared molecular line survey of the Orion hot core

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The basic building blocks of life are synthesized in space as part of the natural stellar evolutionary cycle, whereby elements ejected into the interstellar medium by dying stars are incorporated back into the dense clouds, which form the next generation of stars and planets. The formation of stars and planets are fundamental to the evolution of matter in the Universe as complex molecules are created and destroyed during this step. Understanding these processes will allow us to answer "What is the relation between the molecules we see in the ISM and the molecular inventory of Earth and the terrestrial planets in the Solar System?" Measuring and cataloguing the inventory of organic molecules and understanding their evolution requires observations over a broad wavelength range (IR, MIR, FIR, (sub)mm, and radio) to cover all stages of this evolutionary cycle needed to link interstellar material to that delivered to planets. High-resolution molecular line surveys provide chemical inventories for star forming regions and are essential for studying their chemistry, kinematics and physical conditions. Previous high spectral resolution surveys have been limited to radio, sub-mm and FIR wavelengths; however, Mid-infrared observations are the only way to study symmetric molecules that have no dipole moment and thus cannot be detected in the (sub)mm line surveys from ALMA. Past mid-infrared missions such as ISO and Spitzer had low to moderate resolving power that were only able to link broad features with particular molecular bands and could not resolve the individual rovibrational transitions. JWST will provide exceptional sensitivity in the MIR, but will also not have sufficient spectral resolution, which can lead to confusion in identifying the contribution from strong to moderate strength molecular species.

We present new results from an on-going high resolution (R 60,000) line survey of the Orion hot core between 12.5 - 28.3 μm and 7 - 8 μm, using the EXES instrument on the SOFIA airborne observatory. SOFIA's higher-resolution and smaller beam compared to ISO allows us to spatially and spectrally isolate the emission towards the hot core. This survey will provide the best infrared measurements (to date) of molecular column densities and physical conditions, providing strong constraints on the current chemical network models for star forming regions. This survey will greatly enhance the inventory of resolved line features in the MIR, making it an invaluable reference to be used by the JWST and ALMA scientific communities.

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Structure and spectroscopic properties of imine and amine acetaldehyde: possible interstellar molecules

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A previous theoretical study shows that imine acetaldehyde can be obtained from the reaction between protonated vinyl alcohol and azanone [2]. O-protonated amino acetaldehyde is shown to be a possible product of the reaction between formamide and CH_5^+ [1]. In addition, amino acetaldehyde is considered as a precursor of glycine. Therefore, imine and amine acetaldehyde could be proposed as good molecule candidates to be found in space and could evolve to more complex organic molecules of prebiotic interest. In the present work, we carried out a computational study of the different conformers of imine [3] and amine acetaldehyde. For characterize its conformers we apply a composite approach which considers the extrapolation to the complete basis set (CBS) limit and core-valence (CV) electron correlation corrections at the at the CC level including single and double excitations and a perturbative treatment of triple excitations (CCSD(T)). Four different conformer are located for both, imine and amine acetaldehyde. Vibrational harmonic and anharmonic frequencies and IR intensities are reported at the CCSD level. Interconversion processes between the conformers characterized are studied. The reported, at "spectroscopic" accuracy, stabilities, molecular structures, as well as spectroscopic parameters for the four imine and amine acetaldehyde conformers that could help in their laboratory or astronomical detection.

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Unravelling the mysteries of the Red Rectangle

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The Red Rectangle is one of the most remarkable objects in the sky, particularly from an astrochemical perspective. In addition to a strong display of infrared emission bands from PAHs, emission in the optical region is prominent and of three main types: Extended Red Emission (ERE), Blue Luminescence (BL) and unidentified molecular emission. These molecular bands appear likely to be the emission complement to some of the diffuse interstellar absorption bands; they have been seen in only one other object, the R Coronae Borealis star V854 Centauri. In this work these multi-wavelength observations are brought together through comparison of the spatial distributions and spectral characteristics of the carriers in steps towards a full assignment. A new proposal for the carrier of ERE, graphene oxide, is presented.

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The SOFIA legacy project FEEDBACK

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Massive stars play a key role in the evolution of the interstellar medium (ISM) in galaxies. They "stir" the ISM through various processes such as ionization, stellar winds, radiation pressure, and finally supernova explosions. This mechanical and radiative feedback of massive stars on their environment regulates the physical conditions of the ISM, sets its emission characteristics, and ultimately governs the star formation activity through negative (molecular cloud destruction) and positive (cloud compression) feedback. Understanding the physical processes that regulate the impact of massive stars on their environment is thus a key question in modern astrophysics and a major theme of the Stratospheric Observatory for Far-Infrared astronomy (SOFIA).

I present the first results of the SOFIA legacy project FEEDBACK that was granted 96 hours observing time in 2017 and 2018 in order to map in 11 prominent Galactic star-forming regions the [CII] 158μm line and the [OI] 63μm line (observed in parallel), using the upGREAT heterodyne instrument. We intend to study the interaction of massive stars with their environment in a sample of sources that span a range in stellar characteristics from single OB stars, to small groups of O stars, to rich young stellar clusters, to mini starbursts. With these observations, it is possible to quantify the relationship between star formation activity and energy injection and the negative and positive feedback processes involved, and link that to other measures of activity on scales of individual massive stars, of small stellar groups, and of star clusters

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A principal component analysis of PAH emission in NGC 2023

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NGC 2023 is a bright visual reflection nebula that has prominent emission from Polycyclic Aromatic Hydrocarbons (PAHs) in the mid-infrared. Studies on NGC 2023 in the mid-infrared show considerable variations in their profile shapes, relative band strengths and peak positions. These variations are attributed to the changes in PAH properties such as size, charge state and molecular structure in response to changing physical conditions. Over the past few years, PAH characteristics have been extensively studied in this reflection nebula; however, the relations between the PAH variability and the local physical conditions have yet to be fully established. We aim to determine the physical conditions in NGC 2023, by investigating PAH variability using a statistical technique called Principal Component Analysis. Here, we present the results of a Principal Component Analysis of the flux values of five PAH bands in NGC 2023. We find that with only two parameters, we can reproduce 98 % of the variance in the data. These parameters are related to the density and the UV radiation field.

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SOFIA/FLITECAM and Keck/NIRSPEC 3-micron observations of PAHs in planetary nebulae and star forming regions

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While believed to be formed in the outflows of carbon-rich planetary nebulae (PNs), polycyclic aromatic hydrocarbons (PAHs) are observed in multiple astronomical phenomena, most notably in star forming regions, which has led to their use as a marker for estimating star formation rates in distant galaxies. Understanding the formation environments of PAHs as well as how star-forming region properties affect their emission spectra is therefore essential to multiple aspects of Astrophysics. Studying young PNs and nearby star-forming regions gives a unique opportunity for fully understanding PAH emission, processing and variation that can be used in interpreting extra-galactic PAH spectra. Using ground-based (Lick/FLITECAM and Keck/NIRSPEC) and stratospheric (SOFIA/FLITECAM) observations of the ∼3-5 micron spectra of young planetary nebulae and nearby star-forming regions, we investigate the spatial distribution and spectral variation of the 3.3 micron PAH feature and its associated aliphatic features. We also set limits on the theoretical contribution of the 4.4-4.8 micron deuterated-PAH features and the weak 5.25 micron PAH emission feature.

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A treasure trove finally unlocked: the story of crystalline silicates as told by 3336 Spitzer-IRS galaxy spectra

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We report the detection of crystalline silicates in 791 out of 3336 galaxies included in the Infrared Database of Extragalactic Observables from Spitzer (IDEOS).
Correlation of the strength of the various detected bands with other observables obtained from the same analysis reveals intriguing trends with the silicate strength and other crystalline band strengths.
Our findings force us to pose an intriguing question: why do we not detect crystalline silicate features along diffuse lines of sight in our own galaxy?

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Dynamic modelling of evolution of COMs in hot cores

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One of the most prominent features in the process of the formation of high-mass stars is the development of a hot molecular core. In the early evolutionary stages, a hot molecular core is observed as a deeply embedded object, compact in size ($<$0.05 pc), with high densities ($>10^5$ cm^{-3}) and temperatures ($>$100 K), and with a chemically rich spectrum coming from complex organic molecules (COMs, molecules with 6 or more atoms). With the aim of understanding the process of the formation of massive stars and the coeval chemical evolution, we are presenting a study of the spatio-temporal evolution of COMs in hot cores during the early phase of star formation. We use hydrodynamic simulations of core collapse, which include episodic outflow feedback, produced using the smoothed particle hydrodynamics (SPH) code GANDALF. We extract the density and temperature evolution of SPH particles and feed them in the astro-chemistry code Saptarsy. 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 different gas phase tracers observed in hot cores and look at the effects of the episodic outburst on the chemistry surrounding massive stars. Finally, we use radiative transfer codes such as RADMC-3D and XCLASS to produce synthetic observations and compare the results with real ALMA observations.

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Formation of hydrogenated fullerene molecules

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Carbon containing molecules such as polycyclic aromatic hydrocarbons (PAHs) and fullerenes are thought to play important roles in interstellar chemistry, with the former accounting for in excess of 10% of the galactic carbon. PAHs are widely observed through their infrared emission and are generally accepted as the carriers of the aromatic infrared bands. In the past decade, the interest in interstellar fullerenes has received new focus following the detection of C_60 and C_70 through their infrared emission features in both stellar atmospheres [1] and the diffuse ISM [2]. In addition, there is evidence through high-resolution laboratory spectra that C_60^+ may be a carrier of some of the diffuse interstellar bands (DIBs) [3]. Given the potential for PAHs to react with hydrogen atoms to form superhydrogenated PAHs, providing a catalytic pathway for molecular hydrogen formation, it is important to consider also the reaction between fullerene molecules and atomic H and D.
Using a combination of temperature programmed desorption (TPD) and scanning tunnelling microscopy (STM) measurements we show that C60 adsorbed on a graphite surface will react with gas-phase D-atoms to form deuterated fullerene species up to C60D36. Adsorption of C60 on a D-saturated graphite surface also results in C_60D_x formation, with a complete suppression of D_2 release from graphite sites. Exposure of C_60 to D-atoms leads to a high temperature D_2 desorption signal, beyond that at which complete desorption of the C_60D_x species has occurred. This may result from D-induced cage collapse, resulting the formation of larger defected graphitic products with higher energy binding sites.

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The ethanol tree: possible gas-phase formation routes of glycolaldehyde, acetic acid and formic acid in interstellar medium

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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. More particularly, glycolaldehyde is an important species in this context, especially because it is the simplest sugar-related compound. Indeed, it is thought to be able to be converted into short dipeptides[1] or amino acids[2] and to ease the formation of more complex sugars.[3]
Moreover, its key roles in ISM appear to be also remarkable since it has been detected in Sgr B2[4], in high- and low- mass star forming regions[5] and more recently in shocked regions[6].
In this contribution it is demonstrated, using a computational strategy integrating state-of-the-art electronic structure calculations and kinetic calculations, that the reaction between two widely diffuse species, that are hydroxyethyl radicals and atomic oxygen, can easily account for the formation of, not only glycolaldehyde, but also acetic and formic acids, species that can also be of interest in both prebiotic chemistry and interstellar medium.

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Molecular beam spectroscopy of planar and non-planar polycyclic aromatic hydrocarbons

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Polycyclic Aromatic Hydrocarbons (PAHs) are considered to be a major component of the interstellar carbon inventory. The (photo)chemistry or evolution of PAHs hence governs the carbon chemistry in the interstellar medium (ISM) significantly, yielding new species and playing an important role in processes such as fullerene formation, H2 formation and isotopic fractionation. The PAH family consist of molecules, usually planar, build up from only hydrogen and carbon, combined into fused benzenoid rings. Most of the previous work has focused on planar species. In this work, we aim to study the properties of planar and non-planar neutral PAHs upon UV irradiation and validate theoretical predictions. We use high-resolution spectroscopy techniques on cold molecular beams to measure mass spectra as well as the UV/VIS spectra of small to large neutral PAHs.

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Gas-phase IRPD spectroscopy of the –H fragment of methylated PAHs

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Infrared pre-dissociation (IRPD) spectroscopy has been shown to be a powerful tool in disentangling tropylium and benzylium cations that are formed in the dissociative ionization of toluene [1]. Recent theoretical studies have suggested that the –H fragment of methylated PAH cations could exhibit the same isomerization processes as those involved in the dissociative ionization of toluene, namely a tropylium-like and a benzylium-like species [2]. In addition, an isomerization barrier of 3.5 – 4 eV was calculated between PyrC7+ and PyrCH2+, the two isomers of the fragment of the 1-methylpyrene cation ($C_{17}H_{11}^+$). Methylated PAHs are expected to be abundant in space [3] and the isomerization process might impact their chemical evolution in photodissociation regions. We have started to investigate the fragmentation of the 1-methylpyrene cation at the Free Electron Laser for Infrared eXperiments facility, FELIX, using the FELion 22-pole cryogenic ion trap [4]. We demonstrated the potential of infrared pre-dissociation spectroscopy to disentangle PAH fragment isomers and an IRPD spectrum of PyrCH2+ tagged with Ne has been obtained [4]. In particular, this technique prevents isomerization processes, which might happen in multiple photon dissociation studies. A main result was to observe the benzylium-like species but not the tropylium-like [4]. This could be rationalized by the fact that the former corresponds to the lower energy fragment according to DFT calculations [5]. We are now testing the idea that the formation of the C7 ring may be prevented in the compact pyrene molecule due to strain effects, but could be relaxed in acene species such as 2-methylnaphthalene and 2-methylanthracene.

This presentation will summarize the different results which have been obtained until now.

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