# BOOK OF ABSTRACTS

## Munazza Alam

(Carnegie Earth & Planets Laboratory)

### Mining Metals: Connecting Refractory Abundances in Ultra-hot Jupiters to Formation Location

The enrichment or depletion of refractory and volatile elements in exoplanetary atmospheres is sensitive to formation location in the protoplanetary disk, planetesimal composition and size, total disk mass, and surface density of solids in the disk. Whereas the chemistry of volatiles has long been the focus of disk modeling efforts, the abundance patterns of refractory species have been neglected because they condense into solids in exoplanets cooler than 2000 K. For ultra-hot Jupiters (UHJs; Teq > 2000 K), however, refractories remain in gaseous form – thus also remaining in the observable part of the atmosphere. We present refractory abundance measurements of the UHJ WASP-76b from high-resolution cross-correlation spectroscopy observations taken with Magellan/MIKE (0.3 - 1 microns), which provides a factor of 1.55x improvement in abundance precisions compared to VLT/UVES. We measure the refractory-to-volatile elemental ratio and interpret our observations in the context of a protoplanetary disk model for refractory elemental condensation sequences at distances between 1–5 AU, assuming chemical equilibrium at these radii. Refractory elements form interior to the water snowline (<3 AU), so the condensation sequences of these species can provide a detailed probe of atmospheric abundances for planets that formed within a few AU. These observations lay the groundwork for tracing the refractory condensation sequence of the hottest gas giants to constrain where and how these planets formed.

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## Felipe Alarcón

(University of Michigan)

### Atomic Carbon as a tracer of hidden flows and a kinematic anomaly in the HD 163296 disk

Over the last five years, a handful of protoplanets have been discovered by measuring the kinematical deviations they produced on their host disk, or by the detection of a circumplanetary disk emission. HD 163296 stands out as one of the best studied protoplanetary disks containing multiple dust substructures hinting at an active and ongoing planet formation. We present the detection of a CI kinematic anomaly in the HD163296 disk located in the deepest dust gap of the disk that is not observed in molecular emission. The anomaly shows prominent redshifted emission with a 1-2 km/s offset from Keplerian rotation, where the stellar jet is blueshifted. Such localised offset could be tentatively associated to gas infall coming from the atomic upper layers of the disk onto a tentative protoplanet carving the dust gap, meridional flows on a dust-depleted region, or a bipolar outflow. We analyze this feature in the MAPS data as well, showing that is atomic in nature, making CI a unique tracer of hidden flows in protoplanetary disks. The atomic nature of the kinematic anomaly means that there is a localized UV source strong enough to dissociate CO launching it at speeds fast enough to differentiate it from the disk rotation. Even with a conservative approach, a non-Keplerian atomic carbon emission is tracing a localized strong UV field in one of the HD 163296's dust gaps. We explore the chemical effects and main changes in gas composition that an additional UV source has on the gas in a planet-feeding region, the deepest HD 163296 dust gap, by post-processing hydrodynamical simulations with chemistry and radiative transfer models. Understanding the chemical evolution of the gas surrounding a nascent planet will provide us with further constrains of the gas composition in planet-forming regions.

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VERONICA ALLEN
(Kapteyn Astronomical Institute)

### Sulfur's journey from the volcanoes of Io

Jupiter's moon Io is the most volcanic object in the solar system, emitting hundreds to thousands of kilograms-per-second of SO2 and other volcanic gases into Io's near space environment. The material spreads - via diffusion, charge exchange and other processes - to make up a complex neutral cloud that forms a torus around Jupiter, centered along Io's orbit. The SO2 dissociates into various states of ionized SO, sulfur, and oxygen atoms. The ionized material is picked up to co-rotate with Jupiter's magnetic field, forming a torus of relatively fast-moving plasma. We have obtained ACA observations of Io's torus targeting sulfur-bearing molecules and our preliminary results provide insight on its extent and composition. With further analysis we aim to trace the transport of sulfur to the ocean moon Europa.

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ELIZABETH ARTUR DE LA VILLARMOIS
(Instituto de Astrofísica, Pontificia Universidad Católica de Chile)

### The physical properties of accretion shocks in a young protostellar system

In the process of low-mass star formation, a protoplanetary disk is assembled around the young star and planets will form within this disk. Therefore, the chemical composition of the early disk is crucial for the gaseous content of future planetesimals. Some molecular species are believed to survive from the parental cloud to the inner regions of the disk, while others are being destroyed or formed by some physical processes that alter the chemistry of the disk. One important physical process that could potentially reset the chemistry is accretion shocks: material from the envelope falls on the circumstellar disk and produces accretion shocks at the envelope-disk interface. These shocks induce an increase of the dust temperature and species that are locked in grain mantles are released into the gas-phase, affecting the chemical content of the early disk. I will present new ALMA observations of a particular Class I protostar, IRS 44, that shows strong and warm emission of sulphur-related species, in agreement with accretion shocks. The detection and analysis of multiple SO2 and SO molecular lines allow us to conclude that the shocked region is consistent with dense gas and temperatures above 70 K. In addition, high-energy SO2 transitions (Eup $\sim$ 200 K) seem to be the best tracers of accretion shocks. Understanding the physical properties of accretion shock is essential to assess their potential to sublimate other molecular species that, otherwise, will remain locked on dust grains.

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Jaehan Bae
(University of Florida)

**Discovery of a Circumplanetary Disk Candidate in Molecular Line Emission**

I will report the discovery of a circumplanetary disk (CPD) candidate embedded in the circumstellar disk of a T Tauri star at a radial distance of 200 au, isolated via 13CO emission. This is the first instance of CPD detection via gaseous emission capable of tracing the overall CPD mass. The CPD is embedded within an annular gap in the circumstellar disk previously identified using 12CO and near-infrared scattered light observations, and is associated with a velocity kink in 12CO. The coincidence all these features suggests that they have a common origin: an embedded giant planet. I will summarize the size, temperature, and gas/dust mass of the CPD obtained from this observation, and discuss the formation mechanism of the CPD-hosting giant planet on a wide orbit in the framework of gravitational instability and pebble accretion.

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Nadia Balucani
(DCBB - Università di Perugia)

**Gas-phase chemistry in star-forming regions: there is still a lot to understand**

TBD

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Ted Bergin
(University of Michigan)

**Linking Planet Formation to Exoplanet Composition**

TBD

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Jenny Bergner
(University of Chicago)

**Ice processing along the journey from interstellar grains to icy planetesimals**

Dust grains in protoplanetary disks are subject to a variety of dynamical processes like mixing, settling, and drift. As grains move through different regions within the disk, they can sample a range of temperatures and UV fields, driving chemical processing of their icy mantles. To explore this dynamically driven ice processing, we have developed a modeling framework which tracks the ice-phase chemistry on individual dust particles as they are transported through the disk, allowing us to evaluate the chemical outcomes for ensembles of particle trajectories. In this talk, I will describe how we are using this framework to address: how is pristine interstellar material incorporated into comets? How do disk substructures influence the dynamics and ice chemistry of dust grains? And, can interesting cometary molecules be sourced from ice processing during the disk stage? Answering these questions is critical to understanding the journey of volatile material from the interstellar medium to planetesimals, and to interpreting the compositions of icy planetesimals in the solar system.

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Eleonora Bianchi
(Univ. Grenoble Alpes, CNRS, IPAG)

**The early stages of solar-type protostars: the missing evidence of large carbon chains**

In the last few years a striking chemical diversity has been identified around Sun-like protostars. Among a wide range of chemical composition, two extreme cases are hot corinos, enriched in interstellar complex organic molecules (iCOMs) and the Warm Carbon Chain Chemistry sources, enriched of unsaturated small carbon chains. The origin of this chemical diversity is unclear and it may be related to environmental conditions at the epoch of icy dust mantles formation. As a matter of fact, the vast majority of observations dedicated to the chemical exploration of solar-type protostars has been obtained via millimeter wavelength telescopes, where relatively light molecules have their peak of emission. In contrast, the lines of heavy molecules (e.g. chains and rings with more than seven C-atoms) at mm wavelengths are substantially weaker. Their observation would add a key piece to the overall puzzle as they might have a crucial role in the heritage of organic material from the pre- and proto- stellar phase to the objects of the newly formed planetary system, such as asteroids and comets. We will report the results obtained in a pilot study performed with the Green Bank Telescope (GBT) to observe several crucial C-bearing chains in the 8.0 – 11.5 GHz and 14.0—15.4 GHz frequency ranges, in L1544 and IRAS16293-2422, which are the two archetypes of prestellar core and protostar, respectively. GBT observations reveal an impressive molecular richness of C-chains (e.g. C4H, C6H, HC7N, HC9N, C3S) and a chemical differentiation between the two sources at large angular scales. These results inspired a SKA1-MID Scientific Use case, developed in the framework of the Cradle Of Life working group, and aimed at imaging the spatial distribution of complex carbon species at small angular scale. The synergy between ALMA and SKA will be crucial to reconstruct the whole chemistry of protostellar disks and to understand if large carbon chains and iCOMs coexist in the planet formation region.

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BERTRAM BITSCH
(Max-Planck-Institute for Astronomy (MPIA))

**Can we constrain planet formation from atmospheric abundances?**

While planet formation theories have been traditionally constrained by the masses and orbital distance distributions of exoplanets, we are now entering an era where additionally constraints from planetary atmospheres become available. These constraints are mostly on the C/O, C/H, O/H and water abundance of planets. Classical planet formation scenarios (without pebble evaporation) can only reproduce super-solar atmospheric abundances via the accretion of planetesimals. In these models, sub-solar atmospheric abundances then require no solid accretion, opening the question why certain planets should accrete planetesimals and others should not. In contrast, our model (Schneider & Bitsch 2021a,b) including pebble drift and evaporation in the disc as well as planet growth via pebble and gas accretion while the planets migrates can explain the formation of giant planets with super-solar and sub-solar abundances without additional solid accretion. These differences arise from the formation location of the planet in respect to ice lines, where planets closer in can accrete more evaporated volatiles compared to planets further out. I will highlight how our model can match the measured super-solar atmospheric abundances of tau Böotis b and the measured atmospheric sub-solar abundances of WASP-77A-b and what this implies for their formation history.

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ALICE BOOTH
(Leiden Observatory, Leiden University )

**An asymmetric ice trap in a planet forming disk**

New planetary systems are formed from the dust and gas in the rotating disks around young stars. Observations of these planet-forming disks with the Atacama Large Millimeter Array (ALMA) can be used to learn about the planet-formation process. In particular, ALMA can trace the composition of the volatiles available to forming planets. Complex organic molecules (COMs) are the precursors of prebiotic molecules, thus detecting COMs in disks when planets are actively forming will help us gain more insight into how life originated in our own Solar System. Until recently, detecting COMs in disks has proved difficult as in most systems they are locked up in ices and thus hidden from ALMA. In this talk, I will present ALMA Band 7 observations of the planet-forming disk IRS 48. These data include the first detections of the molecules sulphur monoxide (SO2), nitric oxide (NO), and dimethyl ether (CH3OCH3) in a protoplanetary disk. The presence of these unique molecules in the gas phase can be explained by the thermal sublimation of the disk ices at the edge of the UV irradiated dust cavity showing that dust traps are also ice traps. With the first detection of the largest COM in a disk, and a tentative detection of methyl formate (CH3OCHO), we show that it is possible to trace the full interstellar journey of COMs across the different evolutionary stages of star, disk and planet formation. These results strongly support the inheritance of ices in protoplanetary disks. I will also give a first look at new ALMA cycle 8 observations which target >20 molecules and will further characterise the molecular inventory of the IRS48 system.

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MATTEO BROGI
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**Tapping into the complexity of exoplanet atmospheres with high res-**

**olution spectroscopy**

TBD

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Sandra Brünken
(FELIX Laboratory, Radboud University)

**Spectroscopic evidence of low-temperature polycyclic aromatic hydrocarbon formation**

TBD

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Hayley Bunn
(Max Planck Institute for Extraterrestrial Physics)

**Millimeter/submillimeter spectrum of partially deuterated isotopologues of methyl mercaptan, CH2DSH and CHD2SH** (poster)

Methyl mercaptan, CH3SH, is one of the few complex organic sulphur bearing species detected in the interstellar medium (ISM) and has been detected in both low and high mass star forming regions. [1-5] The further detection of sulphur bearing species in the ISM is required in order to understand their formation and evolution. The level and location of deuteration in complex organic molecules in the ISM act as a tracer for the regions chemical and physical evolution. The millimeter spectrum of the monodeuterated isotopologue of methyl mercaptan, CH3SD, has been previously reported but is yet to be detected in the ISM. [6] The microwave spectra of the partially deuterated isotopologues in the methyl group of methyl mercaptan, CH2DSH and CHD2SH, have been reported for the ground and torsionally excited state providing minimal rotational information for extension up to higher frequencies required for astronomical observation. [7-8] Therefore, additional spectral information is required for their interstellar identification. The detection of deuterated methyl mercaptan in the ISM and the relative abundance of all isotopologues will provide insight into the chemical origin of this simple sulphur species. The collection of the millimeter wave spectrum of CH2DSH and CHD2SH is currently underway in order to provide the necessary spectral information for their detection in the ISM, we will report on the progress of the collection and analysis. 1. R. A. Linke, et al., Astrophys. J. 232, L139–L142 (1979) 2. E. Gibb, et al., Astrophys. J. 545, 309–326 (2000) 3. L. Majumdar, et al., Mon. Not. R. Astron. Soc. 458, 1859–1865 (2016) 4. L. F. Rodríguez-Almeida et al., Astrophys. J. Lett. 912, Art. No. L11 (2021), 5. H. S. P. Müller, et al., Astron. Astrophys. 587, Art. No. A92 (2016) 6. O.

Zakharenko, et al., Astronomy & Astrophysics 621, A114 (2019) 7. C.F. Su, et al., The Journal of chemical physics 79, 12, 5828-5834 (1983) 8. C. F. Su, et al., Journal of Molecular Spectroscopy 158,1, 21-26 (1993)

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Laura Ann Busch
(Max-Planck-Institut fuer Radioastronomie)

### Exposing the COMfort zone of Sgr B2(N1) by resolving the desorption process of complex organic molecules in the hot core

Studying the evolution of complex organic molecules (COMs) across different stages of star formation is a key in understanding their role in the possible prebiotic chemistry of later stellar systems. This is of grave importance now, given the rising number of detections of COMs, and moreover, with increasing complexity. Although progress has been made towards interpreting the nature and evolution of COMs, we still lack knowledge concerning the beginning of the COM's journey in interstellar gas. Many interstellar complex organic molecules (COMs) have first been detected in the vicinity of high- and low-mass protostars at temperatures higher than 100K. The production of many COMs is thought to happen via reactions between radicals on dust grains before the COMs desorb upon heating of the collapsing envelope by the nascent protostar. The characteristic temperature of 100K denotes the point when water, the main constituent of the dust grains' ice mantles, desorbs from the grain surfaces, along with many other species, perhaps including the COMs themselves. This thermal co-desorption process of COMs with water has so far not been observationally confirmed, mainly due to the insufficient angular resolution of astronomical observations. Tackling the question of the COM's arrival in the gas phase is one of the objectives of the ReMoCA (Re-exploring Molecular Complexity with ALMA) survey that targets the massive star-forming region Sagittarius B2 (N) in the Galactic centre region. Thanks to the sub-arcsecond resolution of the survey, we resolve the COM emission in the main hot molecular core Sgr B2(N1) and derive resolved profiles of rotational temperature, column density, and abundance of various COMs. Based on these profiles we resolve the desorption process of COMs in a hot core for the first time. The bulk of the COMs that are (partly) produced on dust grains desorb thermally at temperatures of about 100K likely alongside water. Moreover, we see indications for non-thermal desorption or another thermal desorption process at lower temperatures.

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Jenny Calahan
(University of Michigan)

### The Chemistry of Planet Formation Revealed

A long-lived carbon and nitrogen-rich chemistry at cold temperatures (¡ 50K) is observed to exist within planet-forming disks as evidenced by bright emission from radicals and small organic molecules in systems with ages between 1-10 Myr. These organics exist near or within in the disk midplane, at temperatures well below their sublimation point and should not be present in the gas. Long-standing traditional models suggest that the chemical evolution is powered by ionization sources, typically cosmic-rays or X-rays. Here we report that the chemistry of planet forming disk transitions from a cosmic-ray/X-ray-dominated regime to a UV-dominated photochemical equilibrium, perhaps on timescales of 1Myr. This photo-chemical dominated gas-phase chemistry develops as the dust grains grow and evolve, thereby increasing the gas-to-dust ratio and shifting the gaseous C-to-O ratio ¿1. This long-lived end-stage chemistry thus exists because UV photons penetrate deeper into the disk than previously theorized. This transition marks a shift from early stages where the oxygen-rich gas can influence the composition of rocky planetesimal cores to late stages where carbon-rich gaseous chemistry can influence the composition of material feeding into the rocky cores of planetesimals in which proto-gas giants obtain their atmospheres. The deeper penetration of UV flux has wide reaching effect, including the extension the magnetorotational-unstable region of the disk, potentially powering to mass-accretion within ¿1Myr-old disks.

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Joshua Carder
(University of Virginia)

### Exploring the Astrochemical Reaction Space using Deep Learning

Astrochemical modeling is a key component in understanding the molecular complexity of interstellar environments as it provides extensive clues for studying a suite of astrophysical phenomena, such as star formation and the cycling of material. To match the chemical diversity and complexity made possible by state-of-the-art observatories, modellers must expand their reaction networks: the number of reactions; and newly theorized or experimentally observed chemical processes to explain the observed abundances. In the case where neither theoretical or experimental works exist in the literature, “chemical intuition” is often used to fill in the gaps based on qualitative grounds such as generalizing reactivity and thermochemistry from similar, known molecules. However, these methods require a nontrivial amount of time, resources, and expertise, causing chemical models to fall rapidly behind observations, both in terms of complexity and abundances. To alleviate these roadblocks, we propose a new method for creating and/or expanding astrochemical networks using machine learning—

which has seen widespread usage in other areas of research—to predict reaction products and the corresponding rates as inputs to models. Here, we use large natural language processing algorithms to learn and encode vector representations of chemical reactants, which is subsequently decoded to produce a logits vector that characterizes product channels. And we further train the algorithm to use the encoded vectors to pass through a subsidiary architecture for predicting rate information for calculating rate coefficients in astrochemical models. The fully trained model should then have the ability for predicting information to construct an updated astrochemical network virtually instantaneously by feeding relevant reactants to the model for prediction. Any newly predicted products can be used to iteratively update the reactant list whereby this process will exponentially expand into a more comprehensive reaction network for exploring the chemistry of observed and unobserved molecules. Furthermore, any key reactions discovered could act as a guidance for kinetic studies to further constrain chemical pathways. We will present our initial results in implementing our deep learning architecture with emphasis on modernizing astrochemical modelling.

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Ludmilla Carone
(Institut für Weltramforschung, IWF Graz)

### Cloudy with a hint of magnetic fields - a very short exoplanet atmosphere review

TBD

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Layal Chahine
(Institute Radio Astronomie Millimétrique (IRAM) and Université Grenoble Alpes (UGA))

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

Our Sun was born in a densely packed star cluster, near massive stars whose energetic radiation must have contributed to shaping the evolution of the surrounding environment. In addition, internal irradiation from energetic particles (¿10 MeV), whose imprint is seen today in the products of short-lived radionuclides in meteoritic material, is also known to have occurred during Solar System formation. How does all of this affect the physics and chemistry of the proto-Sun-like objects and their immediate surroundings? How is the material within this region is shaped? Is it altered by internal and/or external processes? A perfect target to answer these questions is OMC-2 FIR4. This is an intermediate-mass protocluster harbouring several protostars. It is located along the Orion Integral Shape Filament,  2 pc north of the Trapezium OB stellar cluster and  0.04 pc south of the protostar HOPS-370, noted for its high velocity outflow. OMC-2 FIR4 is considered as the nearest analogue of the environment in which the Sun may have been born. In this context, we used ALMA observations at 1.3mm to investigate how this protocluster appears at small ( 100-800 au) scales in multiple molecular tracers. We carried out a detailed chemical study on the sun-like protostar HOPS-108, and we detected 11 interstellar Complex Organic Molecules (iCOMs) such as CH3OH, HCOOCH3 and CH3OCH3. Our results can be summarised as follows: (1) significant enhancement of the HCOOCH3 abundance with respect to other hot corinos, (2) a [CH2DOH]/[CH3OH] ratio of  2.5

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## Ko-Ju Chuang

(Leiden Observatory)

### Formation of complex organic molecules in molecular clouds: the top-down mechanism through non-energetic/ energetic processing of C2H2 ice

Interstellar complex organic molecules (COMs) have been identified in various star-forming regions, from translucent clouds to the solar system. The simultaneous detection of these species offers hints of a share chemical history. Besides sugar-relevant species (C2HnO2; glycolaldehyde and ethylene glycol), which have been studied along with the solid-state reaction scheme of CO-H2CO-CH3OH on dust grains, the formation of another group of O-bearing COMs expressed by the formula C2HnO, including ketene (H2CCO), acetaldehyde (CH3CHO), and ethanol (CH3CH2OH), is still under debate. Moreover, observational results often show their appearance well before the so-called catastrophic CO freeze-out stage, suggesting an efficient formation pathway in the interstellar ice is needed. In this work, we experimentally investigate the COM formation through a so-called top-down mechanism that involves non-energetic (thermal) and energetic (non-thermal) processing of unsaturated hydrocarbon C2H2 ice under molecular cloud conditions. The chemical reactions between C2H2 and H atom/OH radical are studied (1) along with H2O formation (i.e., O→OH→H2O) on grain surfaces and (2) in a mixture with H2O bulk ice upon cosmic rays (H+) impact. The ongoing ice chemistry is revealed using IR absorption spectroscopy and complementarily supported by mass spectrometry. Experimental findings show that OH radical addition reactions to C2H2 followed by successive (de-)hydrogenation acting as molecular backbone provides an efficient pathway forming acetaldehyde, vinyl alcohol, ethanol, and ketene. The isomerization from vinyl alcohol to acetaldehyde (enol ¡-¿ keto) through an intramolecular route is found. In the cosmic rays-driven ice chemistry, the temporal evolution of these species is recorded, showing a clear composition transition of the product from H-poor to H-rich species is observed as accumulated energy dose (in star-forming evolution). Furthermore, the top-down mechanism based on C2H2 interacting with NH2 radical and H atom is testified to understand better the icy origin of the (recently) observed N-bearing analogs, including ketenimine (H2CCNH), acetonitrile (CH3CN), vinylamine (CH2CHNH2), acetaldimine (CH3CHNH), and ethylamine (CH3CH2NH2).

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Kathy Chubb
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**Searching for a variety of molecules in exoplanet atmospheres**

TBD

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Ilse Cleeves
(University of Virginia)

**Toward Seeing Both the Protoplanetary Forest and the Tree**

TBD

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Laura Colzi
(Centro de Astrobiología (CSIC-INTA))

**Deuterium Fractionation as a Multiphase Component Tracer in the Galactic Center**

The Central Molecular Zone (CMZ) contains most of the mass of our Galaxy but its star formation rate is one order of magnitude lower than in the Galactic disk. This is likely related to the fact that the bulk of the gas in the CMZ is in a warm (¿100 K) and turbulent phase with little material in the pre-stellar phase. In this talk I will present IRAM 30m and APEX observations of deuterium fractionation (D/H ratios) of HCN, HNC, HCO+, and N2H+ toward the CMZ molecular cloud G+0.693–0.027 (Colzi et al. 2022). These observations clearly show, for the first time, the presence of a colder, denser, and less turbulent narrow component, with a line width of about 9 km s-1, in addition to the warm, less dense, and turbulent broad component with a line width of about 20 km s-1.

For this new component, D/H ratios ¿1e-4 and excitation temperatures of 7 K for all molecules have been found, suggesting kinetic temperatures<30 K and H2 densities ¿ 5e4 cm-3. This new method indicates that the degree of deuteration of different molecules, such as N2H+ and HCO+, and their line profiles can be used to reveal the different gas components in the line of sight to the CMZ. This will allow to identify denser gas that is on the verge of gravitational collapse and that will host future protostars.

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## Alex Cridland

(L'Observatoire de la Cote d'Azur)

### Chemistry in the PDS 70 system and constraints on the formation history of planets b and c

The PDS 70 system is one of only a few stellar system that includes young gas giant planets - effectively finished with their growth stage - as well as the rement of their protoplanetary disk. It thus represents an interesting labratory for testing planet formation theories because it lacks the billion year time gap between disk dispersal and observation that is common in older planetary systems. Here I will present a first test of the core accretion model in predicting the chemical composition of the atmospheres of PDS 70b and PDS 70c. The presented theoretical framework uses molecular line emission observed with ALMA to constrain the current-day disk physical and chemical structure. These constraints are then used to build a physical/chemical model of the protoplanetary disk at an age of 1 Myr - at a time when the planets were in their first stages of their formation. We this model, the gas accretion is computed and the abundance of carbon and oxygen-bearing molecules is predicted. We find that the current observational constraints on the planets (especially c) provide only weak constraints on the planet formation process, but with improved observations both chemical processes in the disk as well as the planets' formation history can be better constrained.

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## Fernando Cruz Sáenz de Miera

(Konkoly Observatory)

### The hot corino-like properties of four FUor-type eruptive young stars

The chemical composition of planets is determined by the material they accrete from the midplane of their parent disks. Thus, understanding the chemical evolution of protostellar/protoplanetary disks is paramount for the study of planet formation. The detection of complex molecules is attainable in the youngest protostars due to their elevated temperatures. However, as the protostars evolve and their disks become colder, the molecules freeze onto the dust grains, becoming harder to detect as evidenced by the low number of Class I and II YSOs with detections of organic molecules. Therefore, the chemical evolution of the protostar, from Class 0 to Class III, remains a mystery. FU Orionis-type objects (FUors) are low-mass young stellar objects experiencing brief periods of enhanced mass accretion rates, which cause an increase in the disk temperature, and, thus, desorb the frozen molecules, making them easier to be detected by current facilities. FUor-type events typically occur in Class I/II objects, i.e. the evolutionary stages when planets are formed, presenting a great opportunity to analyze the chemical composition of disks as they are feeding gas and dust to the protoplanets. Here we present serendipitous detections of complex organic molecules around four FUor-type objects: L1551 IRS 5, Haro 5a IRS, OO Ser and V346 Nor. The molecules detected (e.g. CH3OH, C2H5OH and CH3COCH3), their temperatures and the size of their emitting regions indicate that all four FUors are similar to hot corinos. We calculated the abundances with respect to methanol, and compared with other young stellar objects that are not in outburst and in different stages of stellar evolution. We will discuss similarities and differences between FUors and quiescent sources to see what is the role that outbursts have in the overall picture of chemical evolution. Finally, we will show how these and other less powerful eruptive young stars can provide information on the chemical evolution of protostars.

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Timea Csengeri
(Laboratoire d'astrophysique de Bordeaux)

**Diversity of COMs in the immediate vicinity of high-mass protostars**
(poster)

Most stars form in multiple systems and clusters, especially OB type stars are frequently found in a clustered environment. Yet, the early phase of star and cluster formation is still poorly understood, and little attention has been paid to the complex interplay between the physical processes and the chemical evolution of the gas. The enrichment of the star forming gas in complex organic molecules (COMs) is associated with emerging deeply embedded heating sources, referred to as hot cores. Neither the physical and chemical conditions at the emergence of COMs, nor the diversity of COMs among hot cores is well established. We discuss here the results of a statistical approach to observationally constrain the physical conditions and the diversity of COMs towards hot cores based on the SPARKS survey and the ALMA-IMF Large program. Using a large number of COMs, we uncover a population of sources that are at moderate temperatures, close to the typical sublimation temperatures of COMs at about 100 K, corresponding to the early warm-up phase chemistry. Our results suggest that once thermal desorption starts, protostellar envelopes become enriched in a variety of COMs, such as methanol, ethanol, heavy complex cyanides and formamide, consistent with models where a large fraction of COMs can be formed on the grains which then sublimate to the gas phase due to the onset of protostellar heating. We find that the molecular composition of the gas is well characterised by mainly O-bearing COMs in the early warm-up phase, while heavy complex cyanides trace better the emerging heated gas component, and thus likely probe regions in the immediate vicinity of protostars. We put in context our results with our understanding of the global molecular diversity of hot cores and hot corino like objects.

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## Marta De Simone

(ESO Garching - Germany)

### Tracking the ice mantle history of Solar-type protostars: the NGC 1333 IRAS 4 case

The various discovered exoplanetary systems are very different from each other and from out Solar System. To understand the origin of this diversity, it is crucial to characterize the early stages of their formation, represented by Solar-type Class 0/I protostars. The gaseous chemical content of these objects directly depends on the composition of the dust grain mantles formed before the collapse starts. However, directly retrieving the ice mantle composition is challenging, but it can be done indirectly by observing the major components once they are released into the gas-phase during the warm protostellar stage. In this contribution I will show the results from our VLA observations toward three Class 0 protostars in Perseus/NGC 1333 (IRAS4A1, IRAS4A2, and IRAS4B). We observed several CH3OH and NH3 lines at planet-forming scales ( 300 au) at cm wavelengths in order to derive their abundance ratio. As a first result, we derived a similar NH3/CH3OH abundance ratio in the three protostars. This tells us that they were born from pre-collapse material with similar physical conditions. In order to give insights on the physical conditions of the pre-collapse material, we compared the observed abundance ratios with astrochemical models predictions. We constrained the dust temperature at the time of the mantle formation to be about 17 K, quite warm for a prestellar core at small scales and that coincides with the average temperature of the southern NGC 1333 diffuse cloud. Therefore, a brutal event had to start the collapse early so that the IRAS 4A1, 4A2 and 4B protostars did not experience the usual pre-stellar core phase. This event could be the clash of a bubble with NGC 1333 south, that has previously been evoked in the literature. My contribution will highlight the crucial role of cm observations, combined with state-to-the-art astrochemical models, in retrieving the protostellar ice mantle history and in giving insight on the dynamics of their birth environment. Finally, these results are an important testbed for future upcoming centimeter facilities, as ngVLA and SKA.

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CECILE ENGRAND
(IJCLab Université Paris-Saclay)

### Probing the asteroid-comet continuum with the Rosetta mission and analyses of cosmic dust particles

TBD

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JOAN ENRIQUE ROMERO
(Universitat Autonoma de Barcelona)

### Radical-ice reactivity: formation of ethanol and vinyl alcohol by CCH(gas) + H2O(ice) (poster)

Star forming regions contain a wide variety of complex molecular species, among which interstellar complex organic molecules (iCOMs, 1,2) are of great interest as their formation, destruction and evolution mark the ultimate organic complexity reached in the interstellar medium. There are two "classical" paradigms trying to explain the origin of iCOMs. They either involve the formation of iCOMs in the gas phase, or on the icy mantles of interstellar dust grains as a result of radical-radical barrierless couplings (e.g., CH3 + HCO -¿ CH3CHO). While the latter has received much attention in the last years, it is not as simple as it could look like, as there can be competitive reactions like H-abstractions from one radical to the other (e.g., CH3 + HCO -¿ CH4 + CO), while in some cases, there may be no reaction at all (3,4). In this contribution we test an alternative mechanism based on the reactivity of a gas-phase radical and a component of the ice by means of computational chemistry techniques. We discuss, among others, the effectively barrierless formation of ethanol and vinyl alcohol as a result of the reaction between a gaseous CCH radical with a water molecule from the ice surface (5), what are the limitations of this particular reaction and what are the key steps involved. (1) Herbst, E. and Van Dishoeck, E. W., ARA&A, 47, 427-480, 2009 (2) Ceccarelli C., Viti S., Balucani, N., et al., MNRAS, 476(1), 1371-1383, 2018 (3) Enrique-Romero, J., Ceccarelli, C., Rimola, A., et al., A&A, 655, A9, 2021 (4) Enrique-Romero, J., Rimola, A., Ceccarelli, C., et al, ApJ SS, 259, 2, 2022 (5) Perrero, J., Enrique-Romero, J., Martinez-Bachs, B., et al., ACS Earth Space Chem., 6, 496-511, 2022

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Judit Ferrer Asensio
(Max-Planck-Institute for Extraterrestrial Physics)

**Tracing the contraction of the pre-stellar core L1544 with HC17O+ (1-0) emission.** (poster)

L1544 is a well-studied pre-stellar core in the Taurus Molecular Cloud. Observations towards this source have shown multiple molecular tracers which present a double-peaked line profile. We present here high-sensitivity and high-spectral resolution observations of the three hyperfine components of the J=1-0 rotational transition of HC17O+ towards the dust peak in L1544, which also appear double-peaked. We used the non-local thermodynamic equilibrium (non-LTE) radiative transfer code MOLLIE combined with the molecular abundances derived from a chemical model and new state-of-the-art collisional coefficients to reproduce the observed line profile. The double peaks are due to the contraction motions at densities close to the critical density of the transition (10e5 cm-3) and to the fact that the HCO+ abundance profile decreases toward the center. I will present and discuss our results which have allowed us to gain better understanding of the physical structure of this core on the verge of star formation.

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Rachel Friesen
(University of Toronto)

**Tracing dynamics via chemistry in filaments and cores: TMC-1 and Oph A**

TBD

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Maryvonne Gerin
(Observatoire de Paris)

**Astrophysics meets data science in the Orion B Giant Molecular Cloud** (poster)

The ORION-B project (Outstanding Radio-Imaging of OrioN-B, co-PIs: J. Pety and M. Gerin) is a Large Program of the IRAM 30m telescope that aims to improve the understanding of physical and chemical processes of the interstellar medium by mapping a large fraction of the Orion B molecular cloud (5 square degrees) with a typical resolution of 27” (50 mpc at a distance of 400 pc) and

200 kHz (or 0.6 km s-1 ) over the full 3 mm atmospheric band. In a first study, we showed how tracers of different optical depths like the CO isotopologues allow one to fully trace the molecular medium, from the diffuse envelope to the dense cores, while various chemical tracers can be used to reveal different environments. A clustering algorithm was then applied to the intensities of selected molecular lines, and revealed spatially continuous regions with similar molecular emission properties, corresponding to different regimes of volume density or far-UV illumination. In addition, a global Principal Component Analysis of the line integrated brightnesses revealed that some combination of lines are sensitive to the column density, the density, and the UV field. In a recent study, we go one step further by checking whether/how it is possible to build a quantitative estimate of the H2 column density, based on the molecular emissivity, and valid over a large range of conditions. This is a prerequisite to accurately estimate the mass of the different (potentially velocity separated) components of a giant molecular cloud, in particular its filamentary nature. To quantitatively interpret these results, we use the Cramer Rao Bound (CRB) technique to analyze and estimate the precision on the abundances, excitation temperatures, velocity field and velocity dispersions of the three main CO isotopologues. The fundamental understanding of the gas properties is now further used to probe the filamentary structure, its kinematics and its relationship with the star formation activity.

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KATHARINA GIERS
(Max Planck Institute for Extraterrestrial Physics)

**A comparison of the deuteration in the pre-stellar core L1544 and the protostellar core HH211** (poster)

Deuteration is one of the main chemical processes at work in the very cold conditions of the earliest stages of star formation. Pre-stellar cores show an increase in the deuterium fraction (¿10

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JOSEP M GIRART
(Institut de Ciencies de l'Espai, CSIC; IEEC)

**Magnetically regulated collapse in the B335: The chemical perspective**

B335 is an excellent target for the study of magnetized star formation models, since it has been proposed as an example of protostar where the disk size is set by a magnetically regulated collapse. Here we present ALMA observations of several molecular lines toward B335. We derive the deuteration fraction for the HCO+ and the CO depletion factor. From here we also derive the ionization fraction and cosmic-ray ionization rate. We found high values and, unexpectedly, an increase of ionization fraction and cosmic-ray ionization rate toward the center of the core. We will discuss the possible explanations and consequences of these high values.

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## Tristan Guillot
(Obs. Côte d'Azur)

### Pebble Wave, Disk Photoevaporation and Compositions of the Sun and Giant Planets

TBD

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## Roya Hamedani Golshan
(I. Physikalisches Institut, Universität zu Köln)

### Hot cores with complex chemistry in the LMC Bar

We show results from our ALMA observations of the immediate vicinity of 20 YSOs in the Large Magellanic Cloud (LMC), selected carefully to search for hot molecular cores. Our small (still the largest to date) survey adds to the statistics of physical properties of star forming regions in the LMC with and without detected complex organic molecules (COMs). The 1.2 mm dust continuum images reveal the presence of clusters with different level of fragmentation. We detect 65 1.2 mm compact continuum cores and analyze the spectra of the 31 brightest ones with XCLASS (Möller et al. 2017). A multitude of molecular lines are detected in the spectra of the cores. Prominent are methanol lines that seem to be ubiquitous in our sample, except toward two of the cores. Other molecular lines with high detection rate are CS, SO, SO2, H13CO+, H13CN, HC15N and SiO. More complex molecules such as HDCO, HC3N, CH3CN and NH2CHO and high excitation transitions of SO and SO2 isotopologues are detected only toward a small subset of the cores. With respect to the chemical richness of the cores, , we confirm the detection of four hot cores based on the high temperatures (¿ 100 K). This result is consistent with previous studies (Shimonishi et al. 2016, 2020, Sewilo et al. 2018, 2022) and also increases the number of detected hot cores in the LMC to seven. Six out of seven hot cores detected in the LMC, are located in the Bar region of this galaxy. These hot cores all show emission from COMs, including methanol, methyl cyanide and/or methyl formate. The only hot core in the LMC, with no COMs detection is outside the Bar region, which has a lower metallicity compared to the LMC bar. Investigating the gas, dust and stellar distribution over the LMC, we postulate that a new generation of star formation has been triggered in the higher metallicity regions of the Bar that result in the detection of hot molecular cores with rich chemistry, resembling the ones in the Galaxy.

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CHRISTIANE HELLING
(Space Research Institute, OeAW)

**Global atmosphere gas and cloud chemistry of exoplanets around different host stars**

TBD

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CHIA-JUNG HSU
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**Chemistry and Cores in Cloud Collision** (poster)

The collisions between giant molecular clouds is a promising mechanism to form massive stars and star cluster. To find the evidence of cloud collision, we coupled the cloud collision simulation with a modified network from UCLCHEM to follow the chemical evolution. We studied the correlation between the projected density and the projected chemical abundances. We examined the CO depletion factor to compare with the observational data from IRDC and found that low cosmic-ray ionization rate is needed for certain cloud. In addition, we performed high resolution simulations to study the prestellar cores formed in the cloud collision. We furthermore utilise CASA post-processing the surface density maps to generate their ALMA 1.3mm synthetic observation results. We then use dendrogram to identify cores from the simulations and their corresponding synthetic observations. The derived CMFs are compared with observational data. We also did virial analysis to each cores and found that half of cores from the colliding case are supervirial.

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NATALIA INOSTROZA
(Universidad Autonoma de Chile )

**Methanediol CH2(OH)2 and hydroxymethyl CH2OH+: key organic intermediates on the path to complex organic molecules** (poster)

Ab-initio molecular dynamics simulations were carried out to study the formation pathways to complex organic molecules when a OH+ projectile hit on an interstellar dust grain covered only by methanol molecules. The selected target material is a methanol cluster formed by ten units (CH3OH)10. The focus is on the process where methanediol CH2(OH)2 and hydroxymethyl CH2OH+, both key organic intermediate molecules, were involved in the formation mechanisms of stable complex organic molecules (COMs). Methods: We perform Born-Oppenheimer (ab initio) molecular dynamics (BOMD) simulations under the hybrid functional of Head-Gordon omegaB97X-D. We use the initial kinetic impact energy of 10, 12, 15, 18, 20, and 22 eV. Results: We corroborate that CH2(OH)2 and CH2OH+ are main precursors to form molecules such as methoxymethanol CH3OCH2OH, formyl radical HCO, Criegee biradical CH2OO, formaldehyde H2CO and its elusive HCOH isomer.We discuss the mechanism formation of those complex organic molecules. We compare the formation pathways with previous theoretical results where both key intermediates are present. The pathways in some cases go through CH2(OH)2 or undergo by CH2OH+. Conclusions: We confirm that CH2(OH)2 and CH2OH+ play a key role on the path to the formation of abundant H2CO. These mechanisms can give insight into alternative pathways relevant to understanding experimental processes with key steps within those precursors.

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Shu-ichiro Inutsuka
(Nagoya University)

### Understanding the star formation in filamentary molecular clouds

TBD

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Sergio Ioppolo
(Aarhus University, Denmark)

### Laboratory Ice Astrochemistry in the Era of JWST

Complex organic species are expected to be formed in a variety of interstellar environments at the surface of ice grains by means of a combination of energetic and nonenergetic processing, e.g., photons, electrons, ions, and atoms, respectively. However, to date, many fundamental questions on the physicochemical origin of the observed molecular complexity in space and its link to life on Earth remain unanswered. The recent successful launch, deployment, and calibration of the James Webb Space Telescope (JWST) is a remarkable milestone, marking the onset of a new era for space science, astrophysics, astrochemistry, and astrobiology. The unprecedented combination of JWST and the ground-based Atacama Large Millimeter/submillimeter Array (ALMA) will respectively map and characterize the ice and the gas content of the interstellar medium toward a variety of space environments and physicochemical conditions, revolutionizing our understanding of the star formation process. In my talk, I will review new emerging laboratory techniques that will aid a correct interpretation of observational ice data to help address key questions regarding the complex molecular evolution of star forming regions.

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ALEXEI IVLEV
(MPE)

### Radiolysis and sputtering of CO ice by cosmic rays: Experimental insights into the underlying mechanisms

We present a dedicated experimental study of generic mechanisms controlling radiolysis and sputtering of astrophysical ices due to their bombardment by cosmic ray ions. Such ions are slowed down due to inelastic collisions with bound electrons, resulting in ionization and excitation of ice molecules. We show that the relative contribution of these two mechanisms of energy loss into the radiolysis and sputtering can be probed by selecting ion energies near the peak of the electronic stopping power. In experiments on CO ice irradiation by He ions, a significant asymmetry both in the radiolysis rate and the sputtering yield is observed for pairs of ion energies at two sides of the peak, corresponding to same values of the stopping power. This implies that the stopping power does not solely control these processes, as usually assumed in the literature. Our results suggest that (i) electronic excitations likely represent the most efficient route for radiolysis and sputtering of CO ice, while (ii) the charge state of impinging ions has a negligible effect.

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ARSHIA JACOB
(Johns Hopkins University)

### HyGAL: Characterizing the Galactic ISM with observations of hydrides and other small molecules

One of the fundamental questions in modern astronomy concerns the life cycle of molecular material in the universe and addressing how molecular clouds are formed. Given, that atomic and molecular hydrogen gases form the major components of the neutral interstellar medium (ISM), cloud formation must involve the transition from regions dominated by HI gas to those dominated by H2 gas. While this phase transition is determined by the environmental conditions in the ambient gas it is primarily driven by changes in the pressure or density (or column density). In addition, the chemical transition from gas which is mainly atomic to gas which is mainly molecular is a critical step in initiating the growth of chemical complexity in the ISM both locally and across Galactic scales. Therefore, understanding the processes responsible for this phase transition are crucial. While this topic is highly complex, absorption spectroscopy of hydrides (molecules or molecular ions with a heavy atom covalently bonded to one or more hydrogen atoms) performed over the past decade have provided a wealth of new information about their use as sensitive tracers of the different phases of the ISM. Moreover, being light molecules, the fundamental rotational transitions of these hydrides lie at terahertz frequencies, a frequency window for which SOFIA is the only observatory that can provide access that is almost unhindered by atmospheric absorption. In this talk I will introduce HyGAL, a SOFIA Legacy program aimed to address several questions related to the HI-to-H2 phase transition and star-formation in general using observations of hydrides. This program surveys six hydride molecules- ArH+, OH+, H2O+, SH, OH and CH- and two atomic constituents -C+ and O- within the diffuse ISM by means of absorption-line spectroscopy toward 25 Galactic background continuum by taking advantage of the unique capabilities and high resolution provided by the upGREAT and 4GREAT instruments on board the SOFIA telescope. I will present the first results obtained and illustrate the use of this data in addressing questions, such as (1) What is the distribution of the H2 fraction in the ISM? (2) How does the density of low-energy cosmic-rays vary within in the Galaxy and (3) What is the nature of interstellar turbulence and what mechanisms lead to dissipation?

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Sigurd Jensen
(MPE )

### Matching theory to observations: A 3D physico-chemical model of the pre-stellar core L1544 (poster)

Pre-stellar cores mark the first stage of the star-formation process and hence also the earliest stage on the chemical trail from molecular clouds to planetary systems. There is increasing evidence that the chemistry in protostellar and protoplanetary systems is inherited from the pre-stellar phases (e.g., Cleeves et al. 2014, Jensen et al. 2021). Establishing the chemical inventory of these cores is therefore central to our understanding of the chemistry in young planetary systems. Sub-millimeter observations of the archetypal pre-stellar core L1544 have revealed a complex chemical morphology not currently understood. The emission of carbon-chain molecules peaks opposite of complex organic molecules such as methanol, while both are offset from the dust peak (Spezzano et al. 2017). To understand the chemical morphology and the underlying physical and chemical causes, I will present a new 3D physico-chemical model of pre-stellar cores embedded in a realistic star-forming cloud. The model consists of several components: an underlying physical RAMSES 3D MHD model of a star-forming cloud which is post-processed with two radiative transfer models (dust continuum and molecular line emission) and a state-of-the-art chemical gas-grain model. With this model, we can produce synthetic maps and spectra of the core and compare with the observed characteristics to explore the mechanisms behind the observed chemical structure. I will present the results of this model and discuss how we can understand the current observations and what the implications are for the chemical trail from pre-stellar core to young planets.

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MIWHA JIN
(University of Virginia)

**The efficiency of explosive desorption in cold and quiescent environments** (poster)

The chemical complexity observed in dark clouds implies the higher efficiency of non-thermal desorption mechanisms than previously thought. Many non-thermal desorption mechanisms (e.g. chemical desorption, cosmic-ray induced desorption) have been proposed, but the inclusion of the proposed mechanisms into astrochemical models has not fully explained the observationally inferred chemical abundances yet. Here we revisited one of the proposed non-thermal mechanisms, so-called explosive desorption, to find complementary explanations for such high chemical abundances in cold environments. In this process, the rapid recombination of radicals stored in the ice results in an explosion of the ice mantles, releasing volatiles into gas. We apply this mechanism to a numerical code and explore the parameters that critically affect the desorption efficiency. The respective efficiencies of different non-thermal mechanisms are also assessed in a range of physical conditions.

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JES JØRGENSEN
(Niels Bohr Institute, University of Copenhagen)

**ALMA's view of the complex chemistry and disks around the youngest protostars**

TBD

Hunarpreet Kaur
(FELIX Laboratory, Radboud University)

## A Cryogenic Ion Trap Beamline at FELIX for Astrochemical Studies
(poster)

A Cryogenic Ion Trap Beamline at FELIX for Astrochemical Studies H. Kaur1, A.N. Marimuthu1, D.B. Rap1, K. Steenbakkers1, S. Banhatti2, S. Schlemmer2, B. Redlich1, S. Brünken1 1 FELIX Laboratory, Institute for Molecules and Materials, Radboud University, Nijmegen, The Netherlands 2 I. Physikalisches Institut, Universität zu Köln, Köln, Germany hunarpreet.kaur@ru.nl, sandra.bruenken@ru.nl Reactive molecular ions play a central role in the chemistry of planetary atmospheres and the interstellar medium. Laboratory astrophysics studies on their formation and reaction pathways under astronomically relevant conditions are crucial to interpret astronomical observations and as input for simulations in astrochemical networks. Of similar importance are spectroscopic studies of the often elusive, but essential, ionic reaction partners, intermediates and products that yield fundamental insights on their geometric and electronic structure, and provide spectroscopic signatures needed for their identification in space [1]. Cryogenic ion traps have proven to be ideal tools for studying ion-molecule reactions under controlled conditions and allow for sensitive spectroscopic studies of mass-selected, cold, and isolated molecular ions. Here, we will describe the combination of such a cryogenic 22-pole ion trap instrument with the mid- and far-infrared free electron lasers at the FELIX Laboratory [2]. It allows for wide-range infrared vibrational action-spectroscopy of molecular ions such as hydrocarbon and nitrogen-containing hydrocarbon cations ranging in size from comparatively small systems (three to six atoms) to polycyclic aromatic hydrocarbons. A focus will be on infrared experiments and methods to disentangle the isomeric composition of ionic samples [3], and how we use and extend these methods to investigate isomerization processes in dissociative ionization [4] and isomer-selective reaction kinetics of ion-neutral reactions at astronomically relevant temperatures [5]. [1] B.A. McGuire, O. Asvany, S. Brünken, S. Schlemmer, Nat. Rev. Phys. 2, 402 (2020). [2] P. Jusko, S. Brünken, O. Asvany, S. Thorwirth, A. Stoffels, L. van der Meer, G. Berden, B. Redlich, J. Oomens, S. Schlemmer, Faraday Discuss. 217, 172 (2019); https://www.ru.nl/felix [3] S. Brünken, F. Lipparini, A. Stoffels, P. Jusko, B. Redlich, J. Gauss, S. Schlemmer, J. Phys. Chem. A 123, 8053 (2019); A.N. Marimuthu, D. Sundelin, S. Thorwirth, B. Redlich, W.D. Geppert, S. Brünken, J. Mol. Spectrosc. 374, 111377 (2020); S. Banhatti, J. Palotas, P. Jusko, B. Redlich, J. Oomens, S. Schlemmer, S Brünken, A&A 648, A61 (2021) [4] D.B. Rap, A.N. Marimuthu, B. Redlich, S. Brünken, J. Mol. Spectrosc. 373, 111357 (2020); D.B. Rap, T.J.H.H. van Boxtel, B. Redlich, S. Brünken, J. Phys. Chem. A 126, 2989 (2022); D. Zeh, M. Bast, D.B. Rap, P.C. Schmid, S. Thorwirth, S. Brünken, S. Schlemmer, M. Schäfer, J. Mol. Spectrosc. 378, 111453 (2021). [5] D.B. Rap, J.G.M. Schrauwen, A.N. Marimthu, B. Redlich, S. Brünken, Nat.

Astron., in press (2022).

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KRISTINA ANNA KIPFER
(University of Bern)

## Difficult ice chemistry: Identifying complex molecules in electron irradiated ice with probabilistic data analysis approaches

Ices play an important role in the overall chemistry of space. Ice layers are present on cryogenic interstellar dust grains, icy moons, and Kuiper belt objects. The pristine ices consist mainly out of simple molecules, for example H2O, N2, and CH4 [1, 2]. These ice layers have become of special interest as thermal processing and irradiation of the ices can lead to the formation of more complex molecules, including biomolecules [3,4,5]. Laboratory experiments have shown that the processing of interstellar ice analogues via electrons or UV irradiation produce amino acids [6] or nucleobases [7]. However, analysis and secure identification of molecules proves increasingly difficult as the molecules become larger in size. We simulate ice chemistry with laboratory experiments. Measurements are conducted with the Cryo(L)MS setup. A copper sample holder is placed in a high vacuum chamber (P¡10E-8 mbar) and cooled down to temperatures as low as 4 K using a cryostat. Gas can be injected into the chamber via a leak valve, where it condenses onto the sample holder due to the low temperatures, forming a layer of ice. The temperature of the sample holder is monitored through a diode, attached to a temperature controller, with which the sample holder can be heated via resistive heating. The setup is equipped with an electron gun to process the ice. In this contribution, the results of temperature programmed desorption – mass spectrometry (TPD-MS) measurements of electron irradiated ice mixtures (CH4, H2O, N2) are analyzed. The gas mixtures are deposited at 20 K and subsequently irradiated with 5 keV electrons. During the irradiation, a change in colour of the irradiated spot is observed, suggesting processing of the ice. After the irradiation, a TPD-MS measurement is performed, during which the sample holder is heated from 20 to 300 K with a heating ramp of 2 K/min and the desorption products monitored via a QMS. The TPD-MS results provide information about the desorption temperatures and mass spectrometric “finger prints” of the molecules that are desorbing. However, the analysis of TPD data often proves difficult if multiple co-desorbing species are present, such as is the case for interstellar ice analogues. Characteristic desorption temperatures may be shifted and multiple species and their fragmentation products can contribute to a signal, making identification difficult. We show a probabilistic approach for agnostic molecule detection in order to identify molecules from the TPD data by investigating the ratios of the desorption peaks for different m/z and comparing them to reference data. This routine helps us to identify the irradiation products and therefore the extent of chemical complexity that can be formed in irradiated ices, as well as identify pathways to biomolecules. References [1] Boogert, A.C. Adwin, Perry A. Gerakines, and Douglas C.B. Whittet (2015). “Observations of the Icy Universe”. Annual Review of Astronomy and Astrophysics 53.1, pp. 541–581 [2] Öberg, Karin & Bergin, Edwin. (2020). Astrochemistry and compositions of planetary systems. [3] Abou Mrad, Ninette et al. (May 2016). “Methanol ice VUV photoprocessing: GC-MS analysis of volatile organic compounds”. MNRAS 458.2, pp. 1234–1241 [4] Allamandola, L. J. et al. (1999). “Evolution of interstellar ices.” In: Space science reviews 90 1-2, pp. 219–32 [5] Herbst, Eric and Ewine F. van Dishoeck (Sept. 2009). “Complex Organic Interstellar Molecules”. In: Annual Review of Astronomy and Astrophysics 47.1, pp. 427–480 [6] Padovani, M., D. Galli, and A. E. Glassgold (July 2009). “Cosmic-ray ionization of molecular clouds”. In: AAP 501.2, pp. 619–631 [7] Oba, Y., Takano, Y., Naraoka, H. et al. Nucleobase synthesis in interstellar ices. Nat Commun 10, 4413 (2019). https://doi.org/10.1038/s41467-019-12404-1

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THORSTEN KLEINE
(MPS)

**Meteorite dichotomy and the early history of the Solar System**

TBD

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LAURA KREIDBERG
(MPIA)

**Exoplanet Atmosphere Compositions in the Era of JWST**

TBD

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BEATRICE KULTERER
(Center for Space and Habitability, Universität Bern)

**Constraints on methanol deuteration during the prestellar stage** (poster)

Methanol, the simplest complex organic molecule, and its mono-deuterated isotopologues, CH2DOH and CH3OD, are routinely observed around protostars across the full protostellar mass range. If the deuteration of both of its functional groups is equally efficient, the CH2DOH/CH3OD ratio should be equal to three. Observations paint a different picture. While the ratio exceeds ten in the case of some low-mass protostars, it can drop to unity for high-mass protostars. This has sparked the discussion if this ratio can be used as a proxy for the physical conditions during the process of star formation. Due to the lack of a firm CH3OD detection, this ratio has not been constrained for the prestellar stage yet. A lower limit derived in the well-studied prestellar core L1544 is found to be ten. I will present a chemical model that investigates different formation pathways towards deuterated methanol under prestellar conditions. It combines experimentally derived formation schemes, and takes results from quantum chemical calculations into account to investigate a range of core ages, dust temperatures, and gas densities typical for the prestellar stage. Independent of the applied model, the theoretically expected value of three is not obtained, confirming that the deuteration of the two functional groups of methanol is not equally efficient. Moreover, CH3OD formation is inefficient in the majority of the models, which questions the idea that the CH2DOH/CH3OD ratio is a suitable tracer for the dust temperature at the prestellar stage. In addition, I will show preliminary results of newly obtained observations towards the methanol peak in L1544 with the IRAM 30m and the GBT. The aim of this data set is to get a better observational constraint on the CH2DOH/CH3OD ratio in a prestellar core, and spatially resolve its variation for the first time.

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Thanja Lamberts
(Leiden Institute of Chemistry and Leiden Observatory)

### On the way to complexity in the ISM: carbon-bearing molecules

The space between the starts is far from empty, and, in fact, a large variety of molecules has been already been detected. Gas-phase molecules make up for about 99

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Charles Law
(Center for Astrophysics — Harvard & Smithsonian)

### Tracing the Vertical Structure of Protoplanetary Disks with High Spatial Resolution CO Line Emission Observations

Molecular line emission in protoplanetary disks originates from elevated surface layers above the disk midplanes. Detailed knowledge of this vertical structure is critical in interpreting a variety of observations, including kinematic signals in CO emission, dynamical stellar and disk mass estimates, and signatures of planet-disk interactions. Observations of mid-inclination (30-75 deg) disks offer an opportunity to directly measure the height of bright molecular lines, as the high angular resolution of ALMA allows us to spatially resolve elevated emission above and below the midplane. This not only greatly expands the number of disks whose vertical information can be inferred beyond edge-on sources, but also allows us to map both the radial and vertical disk structure at the same time. Using this approach, we have extracted CO emission surfaces in over ten disks with existing ALMA archival data. This sample nearly triples the number of disks with mapped emission surfaces and confirms the wide diversity in emitting heights (z/r=0.1 to ¿0.5) hinted at in previous studies. Since this sample spans a wide range in stellar mass, age, and disk size, we can assess how source properties influence the vertical gas distribution. Combining our sample with literature sources, including the MAPS disks, we find that CO emitting heights weakly decline with stellar mass and gas temperature, which is consistent with simple scaling relations. We observe a strong positive correlation between CO height and disk size, which is likely due to the flared structure of disks. We also find that CO surfaces trace 2-5 gas pressure scale heights, and we explore the possibility of calibrating emitting surfaces as empirical tracers of disk scale heights. Overall, we show an effective method for extracting CO emitting layers in a large sample of disks and note that such a method can naturally be extended to comparable observations of CO isotopologues, which allow a full mapping of 2D disk structure and temperature, or to other important molecular tracers of disk chemistry and structure.

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HELENA LECOQ MOLINOS
(Space Research Institute, Austrian Academy of Sciences, Graz)

### Simulations of vanadium oxide clusters to constrain their role on cloud nucleation in exoplanets

Clouds are observed in gaseous planets throughout the galaxy. The processes by which these clouds are created are still debated. On rocky planets clouds can form when a super-saturated gas condenses on solid dust particles transferred from the surface to the atmosphere. However, gaseous planets do not have a surface that can provide solid dust particles acting as seed nuclei. Therefore, a phase transition, from gaseous to solid, must take place in order for dust particles, and hence clouds, to form. From a microscopic perspective, this transition is initiated by the clustering of gas molecules to first form nanometer-sized particles (nanoclusters), which can further coagulate to macroscopic dust grains. Nanoclusters can therefore be considered as a bridge between the gas and the solid phase. The formation of nanoclusters is called nucleation. The nature of these nanoclusters that take part in the nucleation process in exoplanet atmospheres, and in particular their potential energies and geometries, as well as their spectral properties, are still not well known. In this work we study vanadium oxides as potential candidates for nucleation in exoplanet atmospheres. We apply a bottom-up approach to obtain global minima candidate structures for multiple vanadium oxide stoichiometries (VxOy)n, with x=1-2, y=1-5, n=1-10, representing the different oxidation states of vanadium oxide compounds. For our large sample of initial cluster geometries, we employ global optimization techniques using multiple parametrizations of the Buckingham-Coulomb pair potential. We then refine our results with quantum mechanical density functional theory (DFT) calculations at the B3LYP/cc-pVTZ level of theory. We conclude that our results are in accordance with the experimental energies listed in the JANAF-NIST tables for vanadium monoxide.

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**Margot Leemker**
(Leiden Observatory, Leiden University)

### Freezing conditions in a warm disk: resolving the 2D snowsurfaces of complex organic molecules

Snowlines, such as the H2O snowline, the CO snowline, and the snowlines of complex organic molecules (COMs) are important locations for the formation of planets as planet formation is thought to be enhanced in their vicinity. Due to the vertical temperature gradient in disks these snowlines are actually snow surfaces. In the era of ALMA with high angular resolution and sensitivity observations we can now resolve the 2D snow surface directly in nearby disks. In this talk, I will present new ALMA observations of molecular lines from the disk surrounding the young outbursting source V883 Ori. The luminosity outburst has heated the disk, shifting the snowlines out to larger radii, 10's of au compared to a ¡=1 au in T Tauri systems, making them now resolvable with ALMA. At these radii the dust disk is optically thin therefore, we can probe all the way down to midplane in this disk. We will use new deep ALMA data to map the 2D snow surfaces of different molecules and compare their locations with their binding energies and excitation temperatures. This will allow us to construct a model-independent 2D temperature structure for the disk. Furthermore, we investigate if these snowlines correlate with changes in the chemical composition of molecules that are in the gas-phase throughout the disk. This will be the first time the 2D snow surfaces of COMs will be resolved in a single disk, directly probing the temperature and chemical composition of the organic planet forming material in a protoplanetary disk.

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**Niels Ligterink**
(Space Research & Planetary Sciences, University of Bern)

### Fundamental parameters for the desorption/adsorption of ice and gas

On many extraterrestrial objects, ranging from interstellar dust grains to icy moons, molecules regularly transfer from ice to gas and vice versa. This directly affects the composition of, for example, Titan's atmosphere or the ice mantles of grains in TW Hya's protoplanetary disk. To understand the conditions under which molecules desorb – or adsorb – knowledge of the objects temperature is not enough, but also the molecular binding energy and pre-exponential factor are required. For many molecules that have been observed in the inter- and circumstellar environment, these parameters have yet to be determined. Laboratory experiments and theoretical studies need to be conducted to find these parameters, but this is time consuming work or can be computationally expensive. Instead, we can also turn to "hidden data" in the literature and employ machine learning to find these parameters. In this contribution, we take a look at a large overview of Temperature Programmed Desorption (TPD) experiments taken from the literature. In some cases these TPD experiments have been used to determine binding energies of molecules, whereas in other cases they have only been used to analyze chemical products. We perform two types of analyses on this dataset. The former data points we use as training data for a machine learning model, which characterizes the molecules in the dataset and uses this information to predict the binding energies of new molecules. On the latter data points we employ transition state theory and the Redhead analysis to determine the relevant binding energies. This work results in a large overview of molecular desorption/adsorption parameters that can be used to determine, among many other things, where molecular snowlines reside in protoplanetary disks or how long it takes for molecules to freeze out from an atmosphere.

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DERYL LONG
(University of Virginia)

### Fasten Your Seatbelts: Constraining Ionization In A Turbulent Disk

Ionization drives critical chemical and dynamical processes within protoplanetary disks. Ions are responsible for important chemical processes, including the formation of organics and water in the cold midplane of the disk. Therefore ionization-driven chemistry is central to the chemical evolution of any planets that may be forming within it. Ionization also has a significant impact on the transport of material throughout the disk via accretion and magnetohydrodynamics (MHD). Sufficient ionization allows the gas to couple to magnetic field lines and in turn drives magneto-rotational instability (MRI). Regions in the midplane in which the disk is not MRI active ("dead zones") are thought to be safe havens for planet formation. Therefore, constraining the ionization fraction throughout a disk is crucial for understanding both possible planet compositions and planet-forming capabilities. We present a forward-modeled 2D ionization map of the DM Tau protoplanetary disk, the first and only known disk with strong turbulence. Using ALMA observations of HCO+, DCO+, N2H+, and H2D+ combined with a grid of 2D chemical models with varying cosmic-ray ionization rates and stellar X-ray spectra, we constrain the ionization fraction throughout the disk. We present our best-fit model and discuss the implications for the physical and chemical mechanisms at play in the enigmatic DM Tau disk.

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F. Long
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### The ALMA High-resolution View of Dust Distribution in Protoplanetary Disks

TBD

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Álvaro López-Gallifa
(Centro de Astrobiología (CAB))

### A comparative study of the chemical content in high- and low-mass star-forming regions and comets

There is growing evidence that our Sun, like most stars, was born in a rich and dense stellar cluster that also contained massive stars. Therefore, the study of the chemical reservoir of galactic massive star-forming regions is crucial to understand the basic chemical ingredients that were available prior the formation of our Solar System, and the subsequent emergence of life. With this purpose, the ALMA project GUAPOS (G31.41+0.31 Unbiased ALMA sPectral Observational Survey) studies the full molecular inventory of the massive star-forming region G31.41+0.31, one of the most chemically rich sources in the Galaxy. In this talk, I will present the results of the comparative study of the abundances of more than 60 different molecules (including complex organic molecules with prebiotic relevance) identified in G31.41+0.31 with those previously derived in other well-studied sources: the low-mass Solar-like protostar IRAS 16293–2422 B, and the comets 67P/Churyumov-Gerasimenko and 46P/Wirtanen. We have used three complementary statistical tests (Spearman, Kendall and Theil-Sen) to study the correlations between the chemical content of these different objects. This comparison gives us important hints about how the chemical complexity of the interstellar medium can be inherited during the process of star and planet formation.

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Jingyi Mah
(Max-Planck-Institut für Astronomie)

**Forming super-Mercuries in disks around metal-rich stars**

Super-Mercuries, rocky exoplanets with bulk iron fraction of more than 60

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Pierre Marchand
(IRAP (Toulouse))

**Protostellar collapse with dust growth**

Dust grains influence many aspects of star formation, including planet formation, opacities for radiative transfer, chemistry, and the magnetic field via Ohmic, Hall, and ambipolar diffusion. The size distribution of the dust grains is the primary characteristic influencing all these aspects. Grain size increases by coagulation throughout the star formation process. I will describe numerical simulations of protostellar collapse using a method recently developed to compute the evolution of the grain size distribution by coagulation at a low numerical cost. We also calculate the non-ideal magnetohydrodynamics effects self-consistently. We find that the coagulation efficiency is mostly affected by the time spent in high-density regions. Starting from sub-micron radii, grains reach 10 $\mu$m in an inner protoplanetary disk that is only 1000 years old. We also show that the growth of grains significantly affects the resistivities, and indirectly the dynamics and angular momentum of the disk

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Bernard Marty
(Université de Lorraine/CRPG)

**Volatile elements on terrestrial planets: an heritage of molecular clouds?**

TBD

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## Andrés Megías

(Centro de Astrobiología (CAB), CSIC-INTA)

### Chemical complexity in pre-stellar cores

Observations carried out toward starless and pre-stellar cores have revealed that complex organic molecules are prevalent in these objects, but it is unclear what chemical processes are involved in their formation. In 2016, Jiménez-Serra et al. observed the L1544 pre-stellar core and found that complex organic molecules are preferentially produced at an intermediate-density shell at radial distances of several 1000 astronomical units with respect to the core center [1]. Later, in 2021, Jiménez-Serra et al. performed similar observations toward the L1498 starless core, believed to be at an earlier stage of evolution than L1544 [2]. In this talk, I will present a related study toward another starless core, L1517B, which could be even younger than L1498 and L1544. L1517B has been observed in the 3 mm atmospheric window using the 30-meter telescope of IRAM at Pico Veleta (Spain), with the aim of determining its level of chemical complexity and to compare it with that of L1544 and L1498. We suggest that the differences between these three cores are due to their evolutionary stage, where the nitrogen-bearing organics are formed first followed by the oxygen-bearing organics once the catastrophic depletion of CO sets in. [1] Jiménez-Serra et al., 2016, ApJL 830 L6. https://doi.org/10.3847/2041-8205/830/1/L6 [2] Jiménez-Serra et al., 2021, ApJ 917 44. https://doi.org/10.3847/1538-4357/ac024c

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## Christoph Mordasini

(University of Bern)

### Extrasolar planets - lessons learned, open questions, and the compositional opportunity

TBD

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## Daniel R. Müller

(University of Bern, Physics Institute, Space Research & Planetary Sciences, Bern, Switzerland)

### High D/H ratios in water and alkanes in comet 67P/Churyumov-Gerasimenko measured with Rosetta/ROSINA DFMS

Isotopic abundances in comets are key to understanding and reconstructing the history and origin of material in the Solar System. Deuterium-to-hydrogen

(D/H) ratios in water have been studied with remote sensing techniques for several comets but no long-term studies of the isotopic compositions of a comet during its passage around the Sun have been reported thus far. Further important molecules with a deuteration that is still poorly understood are linear alkanes. Being the simplest members of the hydrocarbon family, representatives of this group of molecules have been studied on several Solar System bodies but only the upper limits of their isotopic ratios of D/H and 13C/12C are currently available for comets. In this study, a detailed investigation of in-situ data obtained with the Double Focusing Mass Spectrometer (DFMS) as a part of the Rosetta Orbiter Spectrometer for Ion and Neutral Analysis (ROSINA) has been carried out. The ROSINA/DFMS instrument was part of the Rosetta mission following comet 67P/Churyumov-Gerasimenko (hereafter 67P) for more than two years. With data over such a long time span, a thorough analysis of the D/H ratio in water in 67P's coma as a function of cometary activity and spacecraft location above the nucleus has been conducted. In addition, the D/H and 13C/12C ratios of the first four linear alkanes in the coma of 67P have been determined. The D/H ratio from HDO/H2O and the 16O/17O ratio from H216O/H217O remained invariable during 67P's passage around the Sun between 2014 and 2016. All evaluated measurements of the D/H ratio in H2O were compatible within $1\sigma$ with the mean value of 5.01 × 10-4 and its relative variation of 2.0

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## GUILLERMO M. MUÑOZ-CARO

(Centro de Astrobiologia (CAB))

### UV and X-ray processing of ice mantles in planet-forming disks: Photodesorption of species and COMs formation

TBD

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## DAVID NAVARRO ALMAIDA

(Observatorio Astronómico Nacional)

### Linking dust and chemical evolution: Taurus and Perseus

The paradigm of the star formation process suffered a dramatic change with the Spitzer and Herschel infrared space telescopes, revealing networks of filamentary structures where stars are born. Now it is believed that filaments precede the onset of star formation, injecting gas and dust into increasingly denser condensations that we call pre-stellar cores. The detailed knowledge of their physical and chemical properties is therefore crucial to understand the star formation process. In this process, many changes take place involving chemistry and dust evolution. The depletion of CO onto grain surfaces leads to deuterium fractionation, increasing the abundance of deuterated molecules, relative to their hydrogenated counterparts, much higher than the D/H ratio. This makes deuterated compounds ideal to trace the dense and cold gas. The deuterium fraction has also been used as a chemical clock, working as an indicator of the evolutionary stage of star-forming sites. Dust properties also change during the star formation process. In dense regions, dust grains are covered by ice mantles that make them sticky, favoring grain coagulation and changing the dust size distribution. Since dust carries the bulk of the cooling radiation during collapse, knowing the dust size distributions is crucial for a better understanding of the star formation process. Taking all this into account, we present a study of deuterated species in pre-stellar/starless cores in Taurus and Perseus using the newest collisional coefficients for HCN, DCN, isomers, and isotopologues, providing the most up-to-date chemical characterization of these sources. Our results allow us to establish evolutionary hierarchies in different environments with different star formation regimes. Given the changes in the dust size distribution occurring in the evolution of a pre-stellar/starless core and the measurable effects in the dust emissivity they have, we measured the 3 mm dust continuum emission coming from the cores with the MUSTANG2 instrument at the Green Bank Telescope. This continuum data allowed us to compute and correlate the variations of the spectral index of the different targets with the chemical evolution. These results help us disentangle the complex interplay between gas chemistry and grain evolution in a collapsing core.

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Teresa Paneque-Carreño
(ESO/Leiden)

### Vertical stratification of molecules in protoplanetary disks: testing disk chemistry models

High spatial and spectral resolution ALMA observations of moderately inclined disks allow us to directly trace the emission location of various molecules in 3D. Through this innovative analysis it is possible to trace perturbations and structure in the azimuthal, radial and vertical distribution. As line emission is closely linked to temperature, density and radiation conditions we can use the observational constraints on the location of a given line to study all of these aspects in protoplanetary disks. In this talk I will present our results on the determination of the vertical distribution of multiple molecules (CO isotopologues, HCN, CN, H2CO, HCO+, C2H) in a sample of 7 disks. The varied morphology of the vertical structure between systems allows us to understand some of the physical properties of each source. In some cases the CO surface can be used to infer the gas pressure scale height of a disk. CO isotopologues also show perturbations in the vertical distribution that are correlated with gaps in the millimetre continuum and kinematical perturbations. Other tracers, such as CN, give us information on the UV radiation affecting the disk material and through the location of H2CO we may be tracing different formation pathways. We compare our observational results to that of thermo chemical models (DALI).

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Jamila Pegues
(Postdoctoral Fellow, Space Telescope Science Institute)

### Models of Protoplanetary Disk Chemistry across the Stellar Spectrum

Exoplanets have been discovered around an astonishing assortment of stars. To understand the chemical origins of these exoplanets, astronomers study the chemistry in their dusty precursors: protoplanetary disks. Observational studies have recently probed volatile disk chemistry around stars across the pre-main-sequence spectrum, from cool M-stars, to familiar solar-type stars, to bright Herbig Ae stars. These studies suggested that differences in the stellar radiation fields could explain the differences seen in the disks' chemistry. At the same time, new studies have detected emission from complex organics in disks around hot stars, and concluded that those organics were actually released from ancient ices inherited from a previous evolutionary phase. It is thus unclear how important or uniquely critical stellar radiation truly is in originating the differences in disk chemistry observed around these different stars. We present a theoretical study of the origins of chemical complexity in protoplanetary disks across the pre-main-sequence stellar spectrum. To do so, we build a large suite of astrochemical disk models at fixed increments in stellar mass, for which we compute radiation fields generated from stellar spectra representative of the models' stars. We carefully apply these stellar radiation fields to compute the chemical evolution within each disk model, including through treatment of the UV and X-ray photochemistry and the use of wavelength-dependent photodestructive cross-sections for chemical species as able. Breaking each disk model down into its vertical and observable layers, we measure the robustness of each disk's volatile chemistry per layer to enhancements and depletions in the stellar radiation. For molecules commonly observed and studied in disks, we further map out the radial and vertical proportions of radiation-driven versus inherited chemistry. Ultimately, we spatially quantify the underlying role of radiation in cultivating the assortment of chemistry observed in disks around such a rich variety of stars.

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Giulia Perotti

(Max Planck Institute for Astronomy)

### The JWST MIRI view on ice and gas in the Flying Saucer edge-on disk

Protoplanetary disks (PPDs) represent the evolutionary link between molecular clouds and planets. Knowledge of their molecular inventory is the key to unveil the chemical trail leading to life, yet too few observational constraints of PPDs exist at infrared wavelengths, especially in the mid-IR. This wavelength regime enables to study the emission of molecular hydrogen, PAH, refractory material, and ultimately the absorption of ices in protoplanetary disks. Compared to previous mid-IR facilities, the JWST MIRI instrument offers unprecedented sensitivity, spatial resolution, and spectral coverage. In this occasion, we will present the first JWST MIRI observations of the Flying Saucer, an isolated nearly edge-on disk (i¿86 deg) located in the rho Oph dark cloud L1688. We will reveal the chemical composition of the gas and solid-state material forming this iconic disk at a resolution it was never observed before. In particular, we will probe the inner disk composition (¡ 10 AU) and present JWST MIRI MRS 5-28 µm spectra of the upper disk surface, confirming or not Spitzer tentative molecular hydrogen and PAH line detections. In tandem with high-resolution archival ALMA data, we will be able to link the astrochemical processes leading to the inner disk composition of the Flying Saucer with the molecular stratification observed in the outer disk.

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## Linda Podio

(INAF - Osservatorio Astrofisico di Arcetri)

### ALMA-DOT: the ALMA chemical survey of Disk-Outflow sources in Taurus

ALMA revolutionised our comprehension of planet formation. The first breakthrough was delivered by the impacting image of the rings and gaps in the disk of HL Tau, suggesting that planet formation occurs early, in disks of less than 1 Myr. ALMA is also revolutionising our comprehension of the disk chemistry, which is crucial to answer another key question about planet formation: what chemical composition planets inherit from their natal environment? Answering this question is the goal of the ALMA chemical survey of Disk-Outflow sources in Taurus (ALMA-DOT). ALMA-DOT targets six Class I, early Class II disks (0.1-1 Myr) in molecular tracers: CO, CN, S-bearing, CS, H2CS, SO, SO2, and simple organics, H2CO and CH3OH. The survey allows us to obtain a comprehensive view of the radial distribution of molecules in young disks, to reveal the disk vertical structure with the first image of the “molecular” and “freeze-out” layer, and to derive the molecules gas-phase abundance ratios. These are compared with the abundance ratios in Class 0 and II sources, and in comets, to reconstruct the chemical evolution from protostars to planets. Moreover, ALMA-DOT allows us to investigate how accretion streamers and ejection phenomena may affect the disk mass budget and chemistry. The results obtained by ALMA-DOT are the first step towards the characterisation of the disk chemical evolution and of the molecular heritage delivered to the assembling planets.

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CHRISTIAN RAB
(University Observatory Munich - LMU)

**Impact of energetic particle events on the chemistry of plant-forming disks and their observational signatures** (poster)

High energy ionization sources such as galactic cosmic rays (GCRs), stellar X-rays, extreme UV (EUV) emission and stellar energetic particles (SEPs), associated with coronal mass ejections (CMEs) and frequent superflares, can ionize molecular hydrogen, the most abundant chemical species in the environment of young stars. Therefore, they play an essential role in the chemistry and evolution of planet-forming disks and forming planets. We use the 2D radiation thermo-chemical disk modelling code ProDiMo (PROtoplanetary DIsk MOdel) to simulate the impact of those high-energy ionization sources on the chemistry of embedded (Class I) and planet-forming disks. The model includes X-ray/EUV radiative transfer and uses input from different particle transport models to calculate the individual molecular hydrogen ionization rates. We study the impact on the chemistry via commonly observed ionization tracers such as HCO+ and N2H+, but also carbon chains. We argue that spatially resolved observations of those molecules in the (sub)mm, combined with detailed 2D models, allow for disentangling the contribution of the individual high-energy ionization sources. Such an approach enables us to put constraints on the occurrence rate and nature of CMEs and the origin of local energetic particle acceleration (e.g. jets, stellar surface). Our model covers the embedded and T Tauri phase of planet-forming disks and can produce synthetic observables for various instruments. This allows us to identify observational signatures that can trace high-energy events during the planet formation period and investigate their impact on the chemical evolution of disks and their importance on the composition of planetary atmospheres.

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MARTIN DOMENECH RAFAEL
(Center for Astrophysics — Harvard & Smithsonian)

**Characterizing the organic chemistry at disk-forming scales in the**

### Serpens molecular cloud

Planets are assembled in disks of gas and dust around forming protostars. Studying the chemistry of the star-forming regions at disk-forming scales is thus paramount to understand how planets obtain their chemical composition. The presence of complex organic molecules (COMs) is of particular importance, because COMs are believed to be the precursors of yet more complex prebiotic species that could participate in the origin of life if delivered to the surface of planets with appropriate conditions. Recently, evidence of early planet formation found in Class I and borderline Class I/II sources (see, e.g., Segura-Cox et al. 2020) have triggered an increased interest in the chemistry at the earliest stages of star formation, the so called Class 0 and Class I sources. In this talk I will present ALMA observations aimed at the characterization of the chemistry at disk-forming scales in six Class 0 and Class I sources located in the Serpens molecular cloud. The observed sources were all candidates to harbor a protostellar disk according to previous continuum emission observations. We detected COM chemistry toward four of the sources. These four sources included Ser-emb 1 (Martin-Domenech et al. 2019) , that presented evidence of rotation at compact scales in the detected molecular emission; and Ser-emb 11 (Martin-Domenech et al. 2021) and 17 (Bergner et al. 2019), two of the only four Class I sources where organic chemistry have been detected at compact scales thus far. This allowed us to compare the organic composition of Class O and Class I sources, and study the evolution of the chemistry during the earliest stages of star-formation.

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SEAN REYMOND
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### Building the Solar System: constrained accretion of the planets

TBD

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VÍCTOR M. RIVILLA
(Centro de Astrobiología (CSIC-INTA))

### Molecular precursors of the RNA-world in the interstellar medium: the chemical mine found in G+0.693-0.027

We still do not understand how simple molecules combine together on early Earth to form large molecules essential for living organisms. Recent prebiotic experiments, based on the RNA-world hypothesis for the origin of Life, have suggested that the three basic macromolecular systems (nucleic acids, proteins and lipids) could have formed from relatively simple molecular precursors. The detection of some of these molecules in space, thanks to the unprecedented capabilities of current astronomical facilities, has opened a new window for astrobiology from the astrochemical point of view. In this talk I will present an overview of the most recent results of an ultradeep unbiased spectral survey towards the Galactic Center molecular cloud G+0.693-0.027 with the Yebes 40m, IRAM 30m and APEX telescopes. Among the more than 125 molecules detected, we have discovered in the last three years 13 new interstellar species towards this cloud . This rich chemical reservoir include key precursors of RNA nucleotides such as hydroxylamine (NH2OH), cyanomethanimine (HNCHCN), glycolonitrile (HCOCH2CN), or urea (NH2CONH2); of sugars, such as the glycolaldehyde isomer 1,2-ethenediol ((CHOH)2); of proteins, such as ethyl isocyanate (C2H5NCO) and propargylimine (HCCCHNH); of lipids, such as ethanolamine (NH2CH2CH2OH) and propanol (CH3CH2CH2OH); and new species with phosphorus, such as the ion PO+. I will summarise all these detections, and I will discuss how these molecules can be formed in the interstellar medium, using newly developed quantum chemical calculations of gas-phase and grain-surface chemistry. This amazing chemical complexity, which might be only the tip of the iceberg, means that interstellar chemistry offers an extremely rich feedstock for triggering prebiotic chemistry.

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NAMI SAKAI
(RIKEN)

**Challenges toward understanding chemical evolution from envelopes to disks.**

TBD

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DIAN SCHRAUWEN
(FELIX laboratory, Institute of Molecules and Materials, Radboud University)

**Interstellar ices in the lab: probing resonant structural changes due to free electron laser irradiation of interstellar ice analogues** (poster)

Along the wealth of gas-phase molecules detected in the interstellar medium, only 6 molecular species have been detected in the solid state, so far – H2O, CO, CO2, NH3, CH4 and CH3OH in order of abundance [1]. Although proposedly small in number, interstellar ices are postulated to play an important role in interstellar chemistry. The recent launch of the James Webb Space

Telescope (JWST) promises high resolution data sensitive to the morphology, mixing environment and thermal history of interstellar ices and might even lead to the detection of new molecular species in the solid state. The Laboratory Ice Surface Astrophysics (LISA) end station at the free electron laser (FEL) facility FELIX in Nijmegen, the Netherlands, has been designed to investigate the structure of interstellar ice analogues as a result of irradiation with intense mid- and far-infrared FEL light. Not only is infrared irradiation ubiquitous in space, but the effect of the vibrational energy on the ice can be linked to the excess energy that can be released in the icy grain, when a chemical reaction has taken place. Understanding how this kind of energy can be taken up and dissipated in structure of an interstellar ice is key in investigating grain-surface reactions. Our experiments so far have shown that ices can restructure upon resonant irradiation. Porous amorphous solid water (pASW) crystallised locally as a result of the release of resonant vibrational energy in the hydrogen-bonding network [2]. Clear restructuring was also observed in amorphous CO2 ices [3]. Recently, we performed a systematic study of mixed ices consisting of H2O and CO2 in ratios between 1:5 (CO2-rich) and 20:1 (H2O-rich). Upon resonant irradiation of the strongest bands of H2O and CO2 in amorphous ices deposited below 20 K, clear restructuring was observed. The irradiation experiments also revealed a strong connection between the components of the mixtures, since irradiation of the H2O band in CO2-rich ices results in restructuring of the CO2-band and irradiation of the CO2 band results in restructuring of the H2O band in H2O-rich ices. To explain these results on a microscopic level, we will employ theoretical simulations [4, 5]. In future experiments we aim expand our studies to layered ices, as well as mixtures of other molecular species of astrochemical relevance. References 1. Boogert, A.C.A., P.A. Gerakines, and D.C.B. Whittet, Observations of the Icy Universe. Annual Review of Astronomy and Astrophysics, 2015. 53(1): p. 541-581. 2. Noble, J.A., et al., Infrared Resonant Vibrationally Induced Restructuring of Amorphous Solid Water. The Journal of Physical Chemistry C, 2020. 124(38): p. 20864-20873. 3. Ioppolo, S., et al., Infrared free-electron laser irradiation of carbon dioxide ice. Journal of Molecular Spectroscopy, 2022. 385. 4. Cuppen, H.M. and E. Herbst, Simulation of the Formation and Morphology of Ice Mantles on Interstellar Grains. The Astrophysical Journal, 2007. 668(1): p. 294-309. 5. Cuppen, H.M. and R.T. Garrod, Modelling of surface chemistry on an inhomogeneous interstellar grain. Astronomy & Astrophysics, 2011. 529.

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Kamber Schwarz
(MPIA)

### Insights into embedded disk chemistry from new models

Recent observations provide growing evidence for rapid physical and chemical evolution during the embedded disk phase. However, interpreting such observations is difficult due to the kinematically complex nature of embedded systems. I will present a new 3D physical/chemical modeling framework for disks embedded in envelopes of infalling gas. I will discuss what these models, when combined with observations, reveal about the likelihood of chemical reset at the disk/envelope boundary as well as the efficiency of chemical processing in embedded disks.

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SAMANTHA SCIBELLI
(University of Arizona)

### Observational Constraints on the Chemical Complexity and Evolution of Low-mass Starless and Prestellar Cores in the Taurus Molecular Cloud

Before a low-mass (M $\leq$ few solar masses) star like our Sun is formed, it is conceived inside a cold ( 10 K) and dense (¿ $10^5$ cm$^{-3}$) region of gas and dust known as starless or dynamically evolved prestellar core. It is essential to study the chemical complexity and evolution of prestellar cores because they set the initial conditions of star and planet formation. In recent years, the detection of complex organic molecules (COMs), any molecule with at least one carbon atom and six total atoms, in prestellar cores has sparked interest in the star formation community due to astrochemical and astrobiological implications. We've found that COMs are prevalent in the L1495 filamentary region of the Taurus Molecular Cloud, from our survey of 31 starless and prestellar cores, spanning a wide range of evolutionary stages, where we detect methanol (CH3OH) in 100

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HALEY SCOLATI
(University of Virginia)

### A Machine Learning Approach to Characterizing the Chemical Inventory of Orion-KL (poster)

The interplay of the chemistry and physics that exists within astrochemically relevant sources can only be fully appreciated if a holistic understanding of their chemical inventories can be gained. Previous work by Lee et al. demonstrated simple regression models can reproduce abundances to help predict new candidate molecules within TMC-1; yet, it remains to be seen to what degree this source is an astrochemical "unicorn" where its simplistic chemistry and physics is readily characterized by simple machine learning models. Unlike TMC-1, the Orion-KL nebula is composed of several structurally distinct environments that differ chemically and kinematically, wherein abundances of molecules between components can have non-linear correlations that can cause the unexpected appearance or even the lack of unlikely species in various environments. Here we present an extension in chemical and physical complexity to the extensively studied hot star forming region of Orion-KL where a proof-of-concept study was performed to assess if classical regression models can accurately reproduce the abundances using the XCLASS chemical inventory. In hopes to gain further insight in the chemical formation and limits of chemical complexity, we employed a hierarchical classification algorithm to identify relationships between environments with respect to the present species. In this talk, we will present results of these machine learning algorithms, as well as their general applicability and interpretability for the study of complex astrochemical environments using Orion-KL as a case study.

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DOMINIQUE SEGURA-COX
(The University of Texas at Austin)

### Embedded Protostars Connect Sizescales and Timescales

TBD

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JAKE SIMON
(Iowa State University)

### Planetesimal Formation in Dust Rings and Implications for Early Planet Formation

How planetesimals form is one of the largest outstanding issues in planetary astronomy. One promising route is a process known as the streaming instability, the end product of which is enhanced concentration of dust grains in the gaseous planet-forming disk. However, even this instability requires an initial enhancement in dust concentration to get started. This initial enhancement may occur in gaseous pressure bumps that slow inwardly drifting dust leading to rings of concentrated dust grains, as have been observed in many protoplanetary systems. Here, I present a series of very high-resolution simulations of grain concentration + streaming instability in these dust rings at stellar distances equivalent to some of the observed dust rings. We find that planetesimal formation via this process is extremely robust for cm-sized grains, but completely fails for mm-sized grains unless the gaseous pressure bumps are sufficiently large in amplitude to completely trap the inwardly drifting grains. However, such large pressure bumps are likely to be themselves unstable and break down into vortices. Furthermore, particle growth models have difficulty producing grain sizes in excess of mm at these distances. Our main conclusion is that either planet-forming disks form grains larger than 1 mm , or planetesimals do not form by the streaming instability in dust rings. This result has a number of important implications for early planet formation, including alternative routes towards planetesimal formation. I will conclude with a brief discussion of these implications.

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ALEXIA SIMON
(Harvard University (PhD Student) )

### Laboratory Experiments on the Entrapment of Hyper-Volatiles in Interstellar and Cometary CO2 and H2O Ice Analogs

Planets and planetesimals acquire their volatiles through ice and gas accretion into protoplanetary disks around young stars. The composition of planets will depend on the distributions of those volatiles (in icy grain mantles and gas) across the disk, which depend on the disk temperature profiles. If the ices are present as a mixture, entrapment of more volatile species in less volatile ice matrices will change the prediction of solid composition, since entrapment allows hyper-volatiles to be present in solid form closer to the star. More recently, we showed that in addition to water, entrapment in CO2 ice may be important for the distribution of volatiles in disks. I would like to present how hyper-volatile entrapment depends on the ice matrix properties, as well as the maximum amount of hyper-volatiles that can be trapped in a given volume of H2O and CO2 ice. Involving a discussion about the implications for the compositions of planet-forming bodies in disk. This work is a laboratory work looking at a range of four hyper-volatiles: CO, N2, CH4 and Ar, each mixed with an ice matrix: H2O and CO2.

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JAN PHILIP SINDEL
(Space Research Institute, Austrian Academy of Sciences, Graz)

### Building cloud condensation nuclei in exoplanet atmospheres - constraining the TiO2 nucleation rate with molecular cluster simulations

The presence of clouds has been detected in many exoplanetary atmospheres, and accurate models of their formation are needed. Cloud condensation nuclei (CCN) are essential in the cloud formation process. On hot Jupiters these condensation seeds are produced through nucleation of highly refractory molecular clusters. In order to calculate nucleation rates, accurate thermo-chemical data of these clusters is needed. This work presents a streamlined approach, combining three levels of complexity to determine the geometries and potential energies of small (TiO2)_N nanoclusters. Experimental data for gaseous TiO2 is used to calibrate the quantum-chemical Density Functional theory (DFT) calculations. The impact of the updated cluster properties on nucleation rates is presented for an example case of a model hot Jupiter atmosphere. Nucleation rates are calculated with modified classical nucleation theory (MCNT) as well as non-classical nucleation theory, with the latter utilising the individual cluster data. It is found that nucleation rates calculated with MCNT are two magnitudes higher when compared to non-classical nucleation approaches. Using the updated thermochemical properties for the clusters, nucleation efficiency for TiO2 drops at a lower temperature, prohibiting nucleation to occur deeper in the atmosphere. Future work includes the extraction of potentially observable spectra for small clusters and the application of this approach to other potentially seed-forming molecules and clusters.

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Olli Sipilä
(Max-Planck-Institut für Extraterrestrische Physik)

**Revised models for cosmic ray-induced desorption in dense clouds**
(poster)

Cosmic rays (CRs) have a large effect on the physical and chemical evolution of star-forming material. A particular aspect of this is desorption; CRs that impact dust grains deposit energy along their track, heating the grain transiently to a higher temperature. The grain then sheds the deposited energy via (partial) desorption of the ice mantle. This mechanism is arguably the most important means of desorbing icy material in regions well shielded from the interstellar radiation field. Earlier models of CR-induced desorption have assumed that the cooling time of a grain following a heating event is constant, based on an assumption that the ice on the grain consists purely of a CO analogue, and that the grains are always heated to a transient maximum temperature of 70 K. In reality, this picture is complicated by two effects: the cooling time depends strongly on the ice composition, and the maximum temperature following an impact is determined by the energy and species of impacting CR. We present the results of new chemical models where we have revised the desorption rates to take into account a cooling time that varies with the mantle composition, and a heating model that takes into account a whole range of different maximum temperatures (with associated frequencies of impact). We find that these revisions to the CR-induced desorption paradigm greatly impact some of the gas-phase molecular abundances. In particular, our time-dependent cooling model predicts that in two-phase chemical models, where the ice is treated as a single reactive layer, gas-phase abundances tend to decrease with respect to the previous models that adopt a constant cooling time. Accurately accounting for the full range of maximum temperatures in turn increases the desorption rates of lightly-bound species like atomic hydrogen, impacting the abundances of molecules that are formed on grain surfaces via hydrogenation.

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Silvia Spezzano
(MPE)

### Nitrogen fractionation across L1544

Isotopologue abundance ratios are the key to understand the evolution of astrophysical objects and ultimately the origins of a planetary system like our own. Being nitrogen a fundamental ingredient of pre-biotic material, understanding its chemistry and inheritance is of fundamental importance to understand the formation of the building blocks of life. We studied the 14N/15N fractionation ratio across a pre-stellar core through IRAM 30m observations of HCN, HNC and CN. Our results show for the first time that the fractionation of nitrogen presents significant variations across a pre-stellar core. The fractionation map that we derived for HCN present a very clear decrease of the 14N/15N ratio towards the southern edge of L1544, the region of L1544 that corresponds to a steeper drop in H2 column density and is consequently more efficiently illuminated by the ISRF (Spezzano et al. 2016). The same trend is tentatively observed also for CN and HNC. Our results strongly suggest that the main fractionation path for Nitrogen in L1544 is the isotopeselective photodissociation. This fractionation mechanisms has so far not been considered for the fractionation of nitrogen towards dense core. 14N15N photodissociate more efficiently than 14N2 because it is not abundant enough to self-shield. The photodissociation of 14N15N is expected to be more efficient towards the more illuminated part of the core, the southern part, where more atomic 15N will be available to form cyanides like HCN, HNC and CN. The effect of isotope-selective photodissociation in Nitrogen fractionation has already been observed towards a protoplanetary disk where the irradiation from UV photons in the inner part of the disk translates into a lower 14N/15N ratio in HCN (Hily-Blant et al. 2019). With our work we show that not only the irradiation of UV photons, but also the uneven illumination from the ISRF onto a pre-stellar core has an effect on the 14N/15N ratio through the isotope-selective photodissociation. We also show that the scatter in the 14N/15N ratio of HCN, HNC and CN observed in dense cores so far might be a consequence of the different illumination on the individual cores, as well as their environment. Pre-stellar cores provide the budget of material that will finally be inherited by forming planets. In order to assess what is the 14N/15N budget that will be inherited from pre-stellar cores, it is important to consider the illumination-induced variations across the core.
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JONATHAN TAN
(Chalmers Univ. and Univ. of Virginia)

**The physics and chemistry of interstellar clouds, filaments and cores**

TBD

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KOTOMI TANIGUCHI
(National Astronomical Observatory of Japan)

**Understanding Chemical Diversity around Massive Young Stellar Objects** (poster)

We present ALMA Band 3 data of carbon-chain species, and oxygen (O)-bearing and nitrogen (N)-bearing complex organic molecules (COMs) toward five massive young stellar objects (MYSOs). Lines of $HC_5N$ and N-bearing COMs have been detected from three MYSOs. The $HC_5N$ emission comes from hot core regions, as well as COMs. We compare observed molecular abundances to results of our chemical simulations, and find that the observed abundances of COMs and $HC_5N$ can be reproduced at the hot-core stage when the temperature reaches 200 K. At this stage, the $HC_5N$ molecules, which are formed in the gas phase and accumulated in ice mantles during the prestellar and warm-up stages, sublimate from dust grains. This is a new type of carbon-chain chemistry occurring in hot regions. We also derive physical parameters of each MYSO by the 2-temperature modified blackbody model, and investigate relationships between chemical compositions and physical parameters. We find that the MYSOs detected in $HC_5N$ and N-bearing COMs are associated with extended hot or warm regions.

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RICHARD TEAGUE
(MIT)

**Towards a six dimensional view of planet formation**

TBD

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LEONARDO TESTI
(ESO/INAF)

**Dust evolution from cores to disks through planet formation**

In this talk I will present current observational evidence and limitations in constraining the evolution of dust properties in disks through the planet formation process. I will discuss our current understanding of the constraints of dust properties in protostellar envelopes from ALMA and VLA observations and the constraints on dust properties through the epoch of planet formation. While optical depth and scattering at millimetre wavelengths have shown to be important concerns in recent years, I will show how multi wavelength high sensitivity surveys allow us to derive general trend. I will show recent evidence that seem to suggest that early planet formation in disks, and the subsequent disk-planet interaction, dominate the evolution of dust in the classical Class II disks.

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KENGO TOMIDA
(Astronomical Institute, Tohoku University)

**High-energy phenomena in protoplanetary disks and their impacts on dynamics and chemistry**

TBD

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ŁUKASZ TYCHONIEC
(European Southern Observatory)

**The first look at protostellar outflows with JWST-MIRI**

Protostellar jets and outflows are key manifestations of an ongoing star formation. They play important role in distributing angular momentum and are directly linked to the accretion process. Studies of jets and outflows at mid-infrared wavelength regime are challenging as this part of the spectrum is effectively blocked by the atmosphere. Yet this is a crucial range to study molecular (especially H2), atomic (e.g., [S I], [O I]), and ionized gas (e.g., [S III], [Fe II]). JWST-MIRI instrument provides orders of magnitude improvement in sensitivity and a large boost in spatial resolution (up to 0.2” at 5 microns) compared to previous instruments in the mid-IR (5-28 micron) range. We present the first low-mass protostellar outflow mapped with JWST-MIRI: BHR71. In this talk, I will focus on the blueshifted side of the outflow powered from the main component of the binary system. With JWST-MIRI IFU we cover 3x3 mosaic (9”x9” at 5 microns). We present initial results showing the distribution of molecular, atomic, and ionized gas across the cavity wall, low-velocity outflow, and the jet. Combined with available ALMA data, we pinpoint the mid-IR tracers mapped with quality never seen before to kinematic components of BHR71 system. Any emission features toward a young, embedded disk will be reported as well. These freshly obtained results will demonstrate the capabilities of MIRI in studies of star formation and synergies with other observatories.

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Maria Teresa Valdivia Mena
(Max Planck Institute for Extraterrestrial Physics)

### Rivers in the sky: streamers discovered towards two Class I sources in Perseus

In the last few years, there has been a rise in the discovery of streamers, which are long gas structures (on the order of 1000-10000 au) that feed the protostellar disk and/or pseudodisk region with material from outside their natal core. This newly observed accretion mechanism goes against the classical picture of star formation, where accretion into the protostar and protoplanetary disk is azimuthally symmetric and relatively isolated from external influences. Streamers have been found in multiple phases of star formation, from the deeply embedded Class 0 phase to the unveiled Class II phase. It is still unclear how these streamers affect the process of mass accretion, in particular beyond the embedded phase, and if (or how) they connect to the large-scale filaments and fibers. In this talk, I will present our results of ALMA and NOEMA observations of 2 Class I protostars (the transition phase between fully embedded and unveiled) in the Perseus Molecular Cloud to follow the flow of material from scales ¿20 000 au ( 0.1 pc), down to the disk scales ( 100 au). We find asymmetric infall signatures towards disk scales in each source, both in agreement with free-fall motion. I will show how we study several molecular line transitions to map the gas kinematics using different molecular tracers and how we interpret these kinematics as free-fall. It is only thanks to this combination of several tracers that enables for a better understanding of the mass delivery process to disk scales. These newfound streamers and asymmetries in the dense core highlight the importance of the local environment beyond the embedded phase of star formation.

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Merel van ’t Hoff
(University of Michigan)

### Searching for Earth's formation conditions: evidence of hot gas around low-mass protostars

Earth is at least two orders of magnitude depleted in carbon with respect to interstellar grains. This means that carbonaceous grains must have been destroyed at the onset of planet formation. A potential mechanism to destroy carbon grains is through thermal sublimation inside the soot line (300-500 K). Chemical signatures of this process being active are an enhancement of nitrogen-bearing complex organics inside the soot line and higher excitation temperatures for these N-bearing molecules compared to oxygen-bearing complex organics that will be uniformly present out to the water snowline (100 K). While such signatures have been observed toward some sources, the current picture is muddled by differences in observational settings. In addition, the number of low-mass protostars with observations available to search for signatures is small. We therefore carried out a pilot survey with NOEMA targeting O- and N-bearing complex organic molecules at 1, 2 and 3 mm toward 7 low mass and 1 intermediate mass protostar. I will present the first results and the first step in determining whether carbon-grain destruction is common at the onset of planet formation; all sources in our sample show evidence of hot (¿ 300 K) gas based on emission from 3 CH3CN K-ladders, including a source with clear signs of a young embedded disk. These observations present the first systematic search for carbon-grain sublimation in low-mass protostars, that is, Earth's formation conditions.

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Martijn van Gelder
(Leiden Observatory)

### Unveiling the ice composition in low-mass protostars with JWST/MIRI

We will present first results on the ice content derived from our JWST/MIRI GTO program on young embedded low-mass protostars. The focus will be on ice features of complex organic molecules (COMs) such as acetaldehyde (CH3CHO) and ethanol (C2H5OH) and sulfur-bearing ices such as SO2, which thus far have only been tentatively detected toward high-mass protostars. These results will mark the first of many constraints on the ice composition toward low-mass protostellar systems. Moreover, the derived ice abundances will be directly compared to the gaseous abundances derived with ALMA for the same sources. The physical conditions in cold (¡15 K) and dark clouds do not allow for efficient gas-phase chemistry. However, atoms and molecules can still stick to the surfaces of dust grains. In turn, this allows for effective chemistry and leads to the formation of molecules ranging from H2O all the way to COMs such as methanol (CH3OH), CH3CHO, and C2H5OH in the ices. When the dust grains move toward the accreting protostar, these ices sublimate, allowing them to be observed in the gas phase with for example ALMA. However, it remains uncertain whether the observed abundance in the gas phase represent those of the ices due to additional gas-phase chemistry in the warmer conditions near the protostar. A more direct way to observe the ice composition is to use infrared absorption features. Through this method, various ices including H2O, CO, CO2, and CH3OH have been detected. However, these studies were limited by the sensitivity of Spitzer or by the Earth's atmosphere for ground-based observations and could therefore only detect the major ice features. The composition of more minor ice species, such as most of the COMs and sulfur-bearing ices, remains poorly constrained. JWST/MIRI will observe the ices at unprecedented resolution and sensitivity in the crucial 5-25 micron range, which is virtually impossible to observe from the Earth, and provide for the first time stringent constraint on the ice composition in young low-mass protostellar systems.

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SERENA VITI
(Leiden University and University College London)

**From clouds to cores: the molecular journey**

TBD

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ABYGAIL WAGGONER
(University of Virginia)

**Observational Evidence of HCO+ Variability in Protoplanetary Disks**

The chemical and physical evolution of planet forming disks is traditionally thought to evolve slowly, over the course of millions of years. However, recent chemical disk models predict that short X-ray flaring events (days) from young stars can drive molecular species to a more complex state. Flare driven chemical pathways are initiated by a rapid and temporary increase in gas-phase cations, such as H3+, HCO+, and H3O+, after a flare event occurs. Observationally catching a flare is challenging, however, and so we present both results from a serendipitous search of data acquired as part of the Molecules At Planet Forming Scales (MAPS) ALMA large program, as well as targeted observations made to follow up previously variable sources with the Submillimeter Array

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SUSANNE WAMPFLER

(Center for Space and Habitability, University of Bern)

**Nitrogen isotopes as fingerprints for the evolutionary history of cosmomaterials from molecular clouds to comets**

Nitrogen isotopes as fingerprints for the evolutionary history of cosmomaterials from molecular clouds to comets Susanne F. Wampfler (1), Kathrin Altwegg (2), Martin Rubin (2), Nora Haenni (2), the ROSINA team, and Jes Jorgensen (3) (1) Center For Space And Habitability, University of Bern, Bern, Switzerland (2) Physikalisches Institut, University of Bern, Bern, Switzerland (3) Niels Bohr Institute, University of Copenhagen, Copenhagen, Denmark Because stars and planetary systems form by a complex interplay of various physical and chemical processes, the resulting planets and minor bodies consist of a mixture of matter that was partially inherited from the natal molecular cloud, and partially reprocessed to various degrees during the protostellar and disk evolutionary stages. Tracing the history of planetary building blocks all the way from the molecular cloud to mature planetary systems is therefore challenging. The stable isotopic ratios of abundant elements such as hydrogen, nitrogen, oxygen, carbon, and sulfur can serve as unique fingerprints for the evolutionary history of cosmomaterials, but require a thorough understanding of the underlying fractionation mechanisms. Owing to its large variations among the solar system bodies and its lower volatility compared to hydrogen, the nitrogen stable isotopic ratio, 14N/15N, is a particularly promising isotopic signature. Even though a lot of progress has been made in recent years in understanding nitrogen isotopic fractionation, there are still a lot of open questions that hamper the use of the 14N/15N as an evolutionary tracer. For instance, while the solar system comets feature 14N/15N ratios that are remarkably constant irrespective of the molecular tracer, the available measurements from prestellar cores, protostars, and protoplanetary disks point toward multiple nitrogen isotopic reservoirs sampled by different nitrogen-bearing species. In this contribution, we will present the nitrogen isotopic ratio of comet 67P/Churyumov-Gerasimenko from in-situ data obtained by the ROSINA double focusing mass spectrometer onboard the Rosetta spacecraft and discuss why identifying the carriers of the isotopic signature is key for shedding light on the apparent discrepancy between comets and star-forming regions. We will also present new measurements of prestellar cores and star-forming regions aiming at resolving the puzzling isotopic composition of NH3 and N2H+ observed in star-forming regions. We will conclude by discussing how the cometary and pre-/protostellar pictures might be reconciled.

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Jason Man Yin Woo
(Observatoire de la Côte d'Azur)

**Terrestrial planet formation from a ring**

The formation process of the terrestrial planets is still a subject of scientific debate. Developing a connection between the early planetesimal formation with the late embryos' giant impact could be a crucial step in settling the debate. In this study, we directly apply the results of planetesimal formation study into high resolution N-body simulations to tackle unsolved problems related to terrestrial planet formation, both on the dynamical and cosmochemical perspective. A recent planetesimal formation study suggested that the terrestrial forming planetesimals could have emerged around the silicate sublimation line at around 1 AU, we therefore revisit an N-body model proposing that all the terrestrial planets originate from a narrow ring of solid material close to the current Earth's orbit (i.e. the ring model). By taking a more fundamental approach of forming the Mars-sized embryos from a ring of planetesimals in our simulations, we found that the embryos formed do not stay in a narrow distribution as the initial conditions adopted by the previous N-body simulations. Such outward diffusive behaviour of the embryo lead to formation of numerous low mass planets from the current Venus-region to the inner edge of the asteroid belt, which does not match with the current architecture of the inner solar system. Our results thus show the importance of including convergent migration so that embryos could stay concentrated around 1 AU as suggested by a recent study. We demonstrate this by adopting a modified gas disc with a surface density peak at 1 AU into our high resolution simulations. Future study should examine how this ring model with convergent migration fits into the context of the isotopic heterogeneity of the inner solar system.

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YAO-LUN YANG
(RIKEN)

### The origin of complex organic molecules in a wide binary Class 0 protostar

Detecting complex organic molecules (COMs) in low-mass protostars starts to become a common practice in the era of high sensitivity interferometry, such as ALMA. Dedicated line surveys unveil the rich chemistry of COMs, suggesting an extensive chemical evolution in the early stage of star formation. However, observations of resolved COM emission are relatively scarce, hindering a direct association with protostellar structures. In this talk, I will present the first result of our high-resolution (20 au) Band 6 ALMA observations of BHR 71, which has two Class 0 protostars separated by 3400 au. We identified several COMs, including CH3OH, CH2DOH, CH3CHO, and CH3C15N, in IRS 1, the main protostar. The COM emission appears as two compact ( 50 au) regions at the north and south of IRS 1, along the outflow direction. Moreover, COM emission in each compact region shows velocity gradients that are consistent with envelope rotation. Based on the morphology and kinematics, these COMs are likely to come from the heated regions at the apex of outflow cavity walls. We also detect COMs in IRS 2 for the first time. We modeled the column densities of COMs with LTE radiative transfer calculations. Interestingly, IRS 2 has a similar CH2DOH column density as the regions in IRS 1, while IRS 2 has only a 10

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YAPENG ZHANG
(Leiden Observatory)

**Isotopologue ratios in exoplanet atmospheres as potential probes of planet formation**

Isotope abundance ratios play an important role in astronomy and planetary sciences, providing insights in the origin and evolution of the Solar System. As we firmly step into the era of exoplanet characterization, detecting isotopologues in their atmospheres becomes feasible, suggesting great potentials of tracing the formation history of planets. In this talk, I will present the first detection of 13CO isotopologue in atmospheres of two young substellar objects, the super-Jupiter YSES-1b and the brown dwarf 2M0355 with medium/high-resolution spectroscopy. The distinct CO isotopologue ratios measured in the atmosphere of the super-Jupiter (12CO/13CO 30) and the brown dwarf (12CO/13CO 100) may hint to their different formation pathways. I will also discuss future prospects of isotopologues in exoplanets, such as measuring isotope ratios of other elements (e.g. oxygen and hydrogen), and benchmarking ratios in planets against stars and brown dwarfs to further exploit the potentials of constraining planet formation.