# From clouds to protoplanetary disks: the astrochemical link

Monday 05 October 2015 - Thursday 08 October 2015

# Hans Harnack Haus Programme

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## Monday 05 October 2015

## FROM CLOUDS TO DENSE CORES (I): Molecular clouds, filaments, dense cores: physical and chemical structure/evolution - (09:00-12:45)

#### Molecular clouds, filaments, dense cores: physical and chemical structure/evolution

#### time [id] title

#### 09:00 [95] Astrochemical Probes From Clouds to Dense Cores

Presenter: Dr. SHIRLEY, Yancy

Recent continuum surveys of the Gould's Belt and the Milky Way have identified tens of thousands of dense cores and clumps within the Galaxy. It is now possible to study all phases of core, clump, and filament evolution before and during star formation with statistically significant samples of objects. Astrochemical processes on these different physical scales provide astrophysical probes of physical conditions as well as a history of evolution. I shall review the physical properties of the hierarchical structure within

molecular clouds - from parsec-scale filamentary structure to dense cores - in the context of these astrophysical processes. Observations of depletion, deuteration, and the evolution of early time vs. late-time chemistry when coupled with the effective excitation densities of different molecular tracers provide crucial information on the kinematic and chemical evolution of cores, clumps, and filaments. I shall highlight the results from recent surveys that have studied these astrochemical processes within the complete dense core populations within nearby molecular clouds.

#### 09:25 [93] The Physical and Chemical Structure of Infrared-Dark Clouds

Presenter: Dr. JIMENEZ-SERRA, Izaskun

Observations at mid-IR and far-IR wavelengths have revealed that the ISM in our Galaxy is highly organised in cold and dense filamentary structures. The most massive of these structures are called Infrared-Dark Clouds (or IRDCs) and are believed to be the initial conditions of massive star and star cluster formation. In the past decade, a large effort has been made to determine the global physical properties of these clouds and of their dense and cold clumps/cores. However, it remains poorly understood how IRDCs form and subsequently fragment into denser sub-structures. In this talk, I will show how molecular line studies of IRDCs have enhance our understanding of the internal physical structure and gas dynamics of these clouds, and how chemistry can be used to distinguish between different scenarios of molecular cloud and star cluster formation.

#### 09:50 [42] Unveiling a Network of Parallel Filaments in the Infrared Dark Cloud G14.225-0.506

#### Presenter: Dr. BUSQUET, Gemma

Filaments are ubiquitous structures in star-forming complexes, which often intersect in high-density regions associated with star formation, know as hub-filament systems. Despite filaments having been recognized more than 30 years ago, the ubiquity of such structures in star-forming regions, which has been recently highlighted by Herschel programs, has brought special attention to their formation mechanism and their role in the star formation process.

What is/are the physical agent(s) responsible of shaping the interstellar material into filamentary structures? How do they evolve? How filamentary structures fragment to form dense cores, and hence form stars?

With the aim of investigating the origin and evolution of filamentary structures and their subsequent fragmentation we started an observational project with different telescopes towards the Infrared Dark Cloud G14.225-0.506, performing a multi-wavelength and multi-scales study of the cloud.

I will present spectroscopic results of the dense gas (e.g. NH\$\_3\$) material of the cloud, which unveil a network of filaments, constituting two hub-filament systems identified using combined interferometric (VLA) and single-dish (Effelsberg) observations (see Figure). This large network of filaments seems to be separated into two main velocity components, separated by 3 km/s, which overlap in the hubs. The two hubs contain the main sites of star formation activity in the cloud, and present a different level of fragmentation, likely due to strong magnetic fields or UV radiation. I will show the main physical/chemical properties of these filaments obtained from a 3mm line survey with the IRAM 30m telescope, and discuss the possible origin of such structures and its relation with the magnetic field.

#### 10:05 [108] Environment and Protostellar Evolution

#### Presenter: Prof. TAN, Jonathan

Even today in our Galaxy, stars form from gas cores in a variety of environments, which may affect the properties of the resulting star and planetary systems. Here, we study the role of pressure, parameterized via ambient clump mass surface density, on protostellar evolution and appearance, focusing on low-mass Sun-like stars and considering a range of conditions from relatively low pressure filaments in Taurus, to intermediate pressures of cluster-forming clumps like the Orion Nebula Cluster, to very high pressures that may be found in the densest infrared dark clouds or in the Galactic center. We present unified analytic and numerical models for the collapse of prestellar cores, accretion disks, protostellar evolution, and bipolar outflows, coupled with radiative transfer calculations and a simple astrochemical model to predict CO gas-phase abundances. Prestellar cores in high-pressure environments are smaller and denser and thus collapse with higher accretion rates and efficiencies, resulting in higher luminosity protostars with more powerful outflows. The protostellar envelope is heated to warmer temperatures, affecting infrared morphologies (and thus classification) and astrochemical processes like CO depletion onto dust grain ice mantles (and thus CO morphologies). These results have general implications for star and planet formation, especially via their effect on astrochemical and dust grain evolution during infall to and through protostellar accretion disks. I discuss some preliminary results of application of more sophisticated astrochemical modeling of these protostellar envelopes, including the effect of environment on deuteration.

#### 10:20 COFFEE BREAK / Poster Viewing / Discussion

#### 11:20 [112] New insights on prestellar cores: deeper and stronger

#### Presenter: Dr. VASTEL, Charlotte

Within the ASAI (Astrochemical Surveys At Iram) Large Program, we conducted an unbiased spectral exploration of a carefully selected sample of template sources, which cover the full formation process of solar-type stars to understand the chemical evolution of the matter during the long process that brought it from prestellar cores and protostars to protoplanetary disks, and ultimately to the bodies of the Solar System.

One of the targeted source is the prototypical prestellar core L1544 on the verge of gravitational collapse (see Caselli et al. 2012 and references within), located in the Taurus molecular cloud complex at d \$\sim\$ 140 pc. The observations were performed using fast Fourier transform spectrometers with a spectral resolution of 50 kHz covering a frequency range between 81 and 110 GHz. The sensitivity of the receivers allowed to push the limits and reach an rms between 3 (lower frequency) and 7 mK (higher frequency). The high sensitivity obtained for those observations led to the surprising detections of many Complex Organic Molecules (COMs) as well as tricarbon monoxide C\$\_3\$O (Vastel et al. 2014). This prestellar core is characterized by a central high-density (2 \$\times\$ 10\$^6\$ cm\$^{-3}\$), low-temperature (\$\sim\$ 7 K), and high CO depletion, accompanied by a large degree of molecular deuteration. Its physical and dynamical structure has recently been reconstructed by Caselli et al. (2012) and Keto et al. (2014) using numerous existing observations toward L1544. Among them, we emphasize the recent detection of water vapor by the Herschel Space Observatory, the first water detection in a prestellar core, which provided key information for reconstructing the physical and chemical structure of L1544. I will present the observations of deuterated water in this core (Quénard et al., 2015).

Based on a multi-line analysis (Vastel et al. 2014) of the methanol lines, we could establish that the detected COMs originate in an outer ring, where UV photons photo-evaporate methanol, whose presence in the gas phase triggers a cold gas-phase chemistry. This is the first evidence that the COMs' chemistry may be driven by the non-thermal desorption of simple ice components, namely, hydrogenated species like methanol and ethene, and not necessarily by other processes such as reactive desorption in which he exothermicity of surface chemical reactions cause the species to be desorbed after their formation (Vasyunin & Herbst 2013).

I will also report the detection of the cyanomethyl radical for the first time in a prototypical prestellar core (Vastel et al., 2015). A complex structure for which we suspected the presence of the hyperfine transitions of the ortho (see Figure 1) and para forms, is observed due to the high spectral resolution of \$\sim\$ 0.1 km/s. We performed computation of all transition frequencies and line intensities for all transitions including satellite hyperfine components for the ortho and para forms of CH\$\_2\$CN at the frequencies observed by ASAI. This is first detection of the fine and hyperfine structure of the ortho and para forms of cyanomethyl radical at \$\sim\$ 101 GHz, resolved in this cold dense core.

Given the key role that the presence of COMs in prestellar cores has in understanding the general mechanisms of their formation, it is of paramount importance (1) to have a census that is as complete as possible of the COMs present in prestellar cores, (2) to better characterize where the COMs' emission comes from in these cold objects, and, as a consequence, (3) to have a better determination of their abundance, at present obtained by dividing the measured species' column density by the total H\$\_2\$ column density of the core.

#### 11:45 [26] The dense core Barnard 1b, a laboratory for star formation studies

Presenter: Prof. GERIN, Maryvonne

The Barnard 1b core in the Perseus molecular cloud is remarkable in several aspects :

\*i)\* It hosts three protostars, including two class 0 sources and a more evolved object. One of the class 0 sources is very young and could still be at the first hydrostatic core stage.

\*ii)\* The core is magnetized with a ratio \$\mu\$ of mass to flux to critical mass to flux between 2 and 10. Protostellar outflows are not aligned with the direction of the ambient magnetic field.

\*iii)\* It shows high abundances of deuterated species, including triply deuterated ammonia and several doubly deuterated molecules and

all main nitrogen species with their \$^{15}\$N isotopologues.

\*iv)\* Organic species are also present including dimethyl ether and methyl mercaptan.

Our team has obtained a high sensitivity line survey of this source (presented in the contribution by N. Marcelino) and deep, high angular resolution observations with NOEMA and with the VLA, which allowed the detection of several new species, and a good characterization of the structure and chemistry of this core, including the two condensations hosting the young protostars and their molecular outflows.

We have derived the \$^{12}\$C/\$^{13}\$C, D/H, \$^{15}\$N/\$^{14}\$N isotopic ratios, constrained the age and evolutionary stage of the protostars and the mass inflow rate.

We show that the properties are consistent with predictions of MHD simulations adapted to the appropriate initial conditions of Barnard1b.

## 12:00 **[46] Dust growth towards disks: self-consistent modelling of dust evolution due to accretion and coagulation** *Presenter: Dr. KOEHLER, Melanie*

What are the properties of dust in the interstellar medium (ISM) and how do these properties change in the transition to denser regions? This is one of the important questions when studying the denser ISM, since dust properties influence, for example, the formation and temperature of the major molecules in molecular clouds and the grain dynamical behaviour when forming protoplanetary disks. It is therefore important to characterise the grain size, structure, shape and material composition in all phases of the ISM.

The observed SEDs of the dense ISM show a decrease in colour temperature, an increase in the spectral index and an increase in emissivity in the far-IR and sub-mm (Juvela et al., 2011, Roy et al., 2013). These variations cannot be explained with environmental differences alone, but are assumed to occur due to changes in the dust properties. We show that these variations can be explained by dust evolution due to accretion and coagulations processes. Our modelling is based on the diffuse-ISM dust model of Jones et al. (2013) and Köhler et al. (2014), for which we allow for the accretion of carbonaceous and ice mantles as well as coagulation into aggregates. We have carried out detailed model calculations using DDA (Draine & Flatau, 2010) in order to derive the optical properties of these evolved grains. Subsequently, we use DustEM (Compiègne et al., 2011) in combination with the CRT radiative transfer code (Juvela et al., 2005) to determine the SEDs which we compare to observations.

The variations in the optical properties due to dust evolution are able to describe the observed changes in the SED from the diffuse to dense ISM with Av<16 (Köhler et al., 2015). With the dust evolution we are able to explain self-consistently the observed variations in colour temperature, spectral index, 250 \$\mu\$m emissivity and mid-infrared emission. We therefore conclude that evolutionary processes and especially grain growth begins in the low-density (diffuse) ISM, which can explain the observed changes in the SED.

Compiègne et al., A&A 525, 103 (2011), Draine & Flatau, ArXiv e-prints 1002.1505 (2010), Jones et al., A&A 558, 62 (2013), Juvela et al., A&A 527, 111 (2011), Juvela, A&A 440, 531, (2005), Köhler et al., A&A 565, 9 (2014), Köhler et al., A&A 579, A10 (2015), Roy et al., ApJ 763, 55 (2013)

#### 12:15 [7] Impulsive spot heating and thermal explosion of interstellar grains revisited

#### Presenter: Dr. IVLEV, Alexei

The problem of impulsive heating of dust grains in cold, dense interstellar clouds is revisited theoretically, with the aim to better understand leading mechanisms of the explosive desorption of icy mantles.

It is rigorously shown that if the heating of a reactive medium occurs within a sufficiently localized spot (e.g., heating of mantles by cosmic rays), then the subsequent thermal evolution is characterized by a single dimensionless number \$\lambda\$. This number identifies a bifurcation between two distinct regimes: When \$\lambda\$ exceeds a critical value (threshold), the heat equation exhibits the explosive solution, i.e., the thermal (chemical) explosion is triggered. Otherwise, thermal diffusion causes the deposited heat to spread over the entire grain -- this regime is commonly known as the whole-grain heating.

The theory allows us to find a critical combination of the physical parameters that govern the explosion of icy mantles due to impulsive spot heating. In particular, the calculations suggest that heavy cosmic ray species (e.g., iron ions) colliding with dust are able to trigger the explosion. Based on the recently calculated local cosmic-ray spectra, the expected rate of the explosive desorption is estimated. The efficiency of the desorption, which in principle affects all solid species independent of their binding energy, is shown to be comparable with other cosmic-ray desorption mechanisms typically considered in the literature. Also, the theory allows us to estimate maximum abundances of reactive species that may be stored in the mantles, which provides important constraints on available astrochemical models.

## 12:30 [39] Modelling the detailed chemical evolution in 3-dimensional, simulations of star forming filaments *Presenter: Dr. SEIFRIED, Daniel*

In the past decades more and more elaborated chemical networks have been developed to describe the chemical conditions of star forming regions under various conditions. However, due to their complexity and high computational demands, they have mainly been applied to one-zone models or static configurations. In contrast, the application to time-dependent, magentohydrodynamical (MHD) simulations has been rather limited.

Here, we present simulations of star forming filaments including one of the largest chemical networks ever used in a fully self-consistent, 3-dimensional, MHD simulation. The simulations are performed with the chemistry package KROME (www.kromepackage.org), for which we have contributed in its development. The KROME package is a highly flexible chemistry solver, which can be adapted to a wide range of astrophysical applications. The network used in our simulations accounts for all relevant cooling and heating processes in the ISM. Moreover, using 40 thoroughly selected species and about 300 reaction rates, this allows us to described the detailed evolution of various important gas tracers like e.g. CO or HCO\$^+\$ as well as the evolution of dust. The chemical network is coupled to a simplified radiation transport scheme allowing us to include photochemical reactions as well.

In our presentation we will discuss the applicability of such large networks in 3D, MHD simulations, in particular with respect to their computational demands as well as the usage on modern supercomputers.

Furthermore, we will present which impact the interstellar radiation field as well as cosmic rays have on the detailed chemical composition during the collapse of filaments. We will also describe the thermal evolution of gas and dust in an unprecedented manner. Both, the chemical evolution as well as the thermodynamical evolution are necessary for producing reliable predictions for modern observations.

In this context we will present synthetic observations of several line transitions and continuum emission produced from our simulation data. We will compare them with actual observations, draw some basic conclusions how to interpret modern observations, and present predictions for future observations.

[Spatial distribution of H, H\_2, C, and CO in a star forming filament][1]

[1]: http://www.astro.uni-koeln.de/~seifried/species.pdf

#### FROM CLOUDS TO DENSE CORES (II): Molecular cloud chemistry; laboratory experiments <u>I. Ions, radicals</u> - (14:00-17:45)

#### molecular cloud chemistry; laboratory experiments I. lons, radicals

time [id] title

#### 14:00 [63] From clouds to dense cores

#### Presenter: Dr. WAKELAM, Valentine

A large fraction of molecules have been observed in cold dark sources. These astronomical objects represent the starting point for the formation of molecules that will participate in the chemistry of the birth of stars and planets. They are also supposed to be the most simple objects in term of physical conditions and history. In this review talk, we will present a summary of the recent model developments that have been undertaken in the last 6 years to reproduce the chemistry in those regions and we will in particular discuss the importance of the formation of these sources and the history of the gas and dust under diffuse conditions.

#### 14:25 [91] High-Resolution Action Spectroscopy of Cold Molecular Ions

Presenter: Dr. BRÜNKEN, Sandra

Molecular ions are important constituents of the interstellar medium. They are major drivers of the chemistry particularly in cold and dense molecular clouds, which are sites of star formation, and are tracers of the physical and chemical conditions in these environments. Their identification in space relies on accurately known transition frequencies provided by laboratory spectroscopy. Conventional absorption spectroscopy has in the past successfully been applied for spectroscopic studies of molecular ions, but is often hampered by low number densities and spectral congestion due to the multitude of species produced at high excitation energies in the discharge cells used for their formation.

These limitations can be overcome by performing experiments on mass-selected ions in cryogenic ion trap instruments. The Cologne laboratory astrophysics group has in the past years developed sensitive action spectroscopic methods based on Laser Induced Reactions (LIR) [1]. For LIR measurements only a few thousand mass-selected ions are stored and cooled in a 22-pole ion trap, and their light-induced excitation is probed by the outcome of an endothermic ion-molecule reaction. Highly accurate ro-vibrational transition frequencies are obtained by using a narrow-bandwidth cw optical parametric oscillator (OPO) calibrated with a frequency comb as excitation source in combination with the cold temperature of the ions [2]. In certain cases even purely rotational transitions have been measured with high-resolution either directly [3] or via a two-photon double-resonance scheme [4]. Very recently, our group used an even more general action spectroscopic scheme based on LIR, which utilizes a change of the rate of ternary He-attachment to the stored, cold ions depending on their internal ro-vibrational or rotational excitation [5,6].

In this talk we will give details on the experimental and methods development for high-resolution ro-vibrational and rotational ion spectroscopy in cryogenic traps. We will also demonstrate the strong interplay of our laboratory work and astrophysical observations with selected examples, e.g. the confirmation of I-C3H+ in photon-dominated regions and the diffuse interstellar medium [6], and the first detection of para-H2D+ in the cold molecular envelope around a young protostellar core [7].

References:

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[6] Brünken, S., Kluge, L., Stoffels, A., Asvany, O., Schlemmer, S., ApJL 783, L4 (2014)

[7] Brünken, S., Sipilä, O., Chambers, E.T., et al., Nature 516, 219 (2014)

#### 14:50 [45] Spin-state chemistry of deuterated ammonia

#### Presenter: Dr. SIPILÄ, Olli

We report on a new gas-grain chemistry model (Sipilä et al. 2015b) that contains multiply deuterated species and separates out the different nuclear spin isomers of molecules with several H and/or D nuclei. The nuclear spin branching ratios are calculated using symmetry rules under the assumption of complete scrambling. The method has been previously used for systems consisting of five H and/or D nuclei by Hugo et al. (2009). The present model is an evolved version of our previous spin-state chemical model (Sipilä et al. 2015a) which included the spin chemistry of hydrogenated species calculated with the formalism of Oka (2004), based on angular momentum algebra applied to nuclear spin statistics.

We apply the model to studying the particular case of (deuterated) ammonia, for which the model predicts that the relative abundances of \$\rm NH\_3\$, \$\rm NH\_2D\$, \$\rm NHD\_2\$, and \$\rm ND\_3\$, as well as their nuclear spin ratios, depend strongly on the kinetic temperature and the gas density. This is illustrated by the attached Figure, where we plot the spin-state ratios of the deuterated forms of ammonia as functions of time at different densities (upper panels) or temperatures (lower panels). According to the present model, the deuteration of ammonia occurs primarily in reactions between \$\rm NH\_3\$ and the deuterated forms of \$\rm H\_3^+\$, i.e., \$\rm H\_2D^+\$, \$\rm D\_2H^+\$, and \$\rm D\_3^+\$.

In cold, dense interstellar cores, the deuterated isotopologs of ammonia are expected to be most abundant toward the center where the density is highest. The spectral lines of the mentioned species are therefore likely to be extremely useful probes of the deep interiors of prestellar cores. The ground-state rotational lines of \$\rm NH\_2D\$, \$\rm NHD\_2\$, and \$\rm ND\_3\$ are observable from the ground (e.g., Roueff et al. 2005). We have recently observed ortho and para \$\rm NH\_2D\$ and \$\rm NHD\_2\$, and meta and para \$\rm ND\_3\$ (no detection for the latter) toward the starless core H-MM1 with APEX (Harju et al. 2015, in prep.), and we find that our new spin-state model reproduces the various abundance ratios well.

References:

Hugo, Asvany & Schlemmer 2009, J. Chem. Phys. 130, 164302

Oka 2004, J.Mol.Spec. 228, 635

Roueff et al. 2005, A&A 438, 585

Sipilä, Caselli & Harju 2015a, A&A 578, A55

Sipilä, Harju, Caselli & Schlemmer 2015b, submitted to A&A

#### 15:05 [19] The Deuteration Clock for Massive Starless Cores

Presenter: KONG, Shuo

Initial conditions are crucial to understanding the formation of massive stars, which is still a mystery. One of the most debated points is whether massive star formation is a fast or slow process. Tan et al. (2013, ApJ, 779, 96, hereafter T13) discovered two massive starless cores C1-N and C1-S with ALMA. Their study suggests \$\sim\$mG magnetic field be present if the cores are virialized. Here we present astrochemical study with observation and modeling. We use deuterium fraction \$D {\rm frac}^{\rm N 2H^+}\$ (\$\equiv\$ [\$\rm N\_2D^+\$]/[\$\rm N\_2H^+\$]) as chemical clock. We utilize the chemical model from Kong et al. (2015, ApJ, 804, 98), and explore the effects of different core collapsing rates relative to free-fall \$\alpha\_{\rm ff}\$  $(\rm d_n_{\rm H}) = \alpha_{\rm H} (\rm H) (\rm$ The chemical network includes spin states, deuterium, and freeze-out. For each \$\alpha\_{\rm ff}\$, we explore models with different initial density, initial depletion, initial ortho-to-para \$\rm H\_2\$ ratio, and cosmic-ray ionization rate. Then we compare output \$D\_{\rm frac}^{\rm N\_2H^+}\$, \${\rm N\_2H^+}\$, and \${\rm o}\$-\${\rm H\_2D^+}\$ with observational results collected from ALMA, CARMA, JCMT, IRAM 30m, and NRO 45m. Multi-transition fitting of \${\rm N\_2D^+}\$ and \${\rm N\_2H^+}\$ lines are performed in order to have the most accurate determination of the deuterium fraction so far possible. Comparisons between the observation and model predictions suggests that both C1-N and C1-S have collapsed at a rate at least 10 times slower than free-fall. This supports the dynamical study in T13, and indicates the potentially important role of magnetic fields in slowing down collapse. Depending on data delivery, we will also present initial results from several ALMA Cycle 2 projects that are related to massive starless cores.

#### 15:20 COFFEE BREAK / Poster Viewing / Discussion

#### 16:20 [105] Gas-phase formation routes of complex organic molecules in the interstellar medium

#### Presenter: Prof. BALUCANI, Nadia

Relatively complex organic molecules (COMs), such as formamide or cyanomethanimine, have been detected in the gas-phase of various regions of the interstellar medium. Some difficulties in assessing their formation routes under the harsh conditions of interstellar objects have progressively brought the current astrochemical models to privilege grain-surface over gas-phase chemistry to explain their formation. In this scenario, grain-surface chemistry is not only responsible for the hydrogenated molecules of the pre-collapse phase, but also for the whole set of the observed COMs (see, for instance, Garrod & Herbst 2006).

Nevertheless, as recently pointed out by a theoretical investigation of two gas-phase reactions leading to formamide and cyanomethanimine (Vazart et al. 2015, Barone et al. 2015), many gas-phase routes have actually been overlooked and not considered in the astrochemical models, while their inclusion with the parameters determined in laboratory experiments or via accurate theoretical calculations could be decisive in reproducing the observed abundances.

In this contribution, we report on recent effort in searching for new formation routes of COMs in the gas-phase by: 1) extensive literature search of previously overlooked bimolecular reactions; 2) testing the new formation routes in astrochemical models. The approach is the same recently used to address the formation of methylformate starting from the parent molecule dimethylether via a set of bimolecular reactions which were studied in laboratory experiments in the 80's but completely ignored in previous astrochemical models (Balucani et al. 2015).

R.T. Garrod and E. Herbst, 2006, A&A, 457, 927

F. Vazart, C. Latouche, D. Skouteris, N. Balucani, V. Barone, 2015, ApJ, in press.

V. Barone, C. Latouche, D. Skouteris, F. Vazart, N. Balucani, B. Lefloch, C. Ceccarelli, MNRAS, submitted.

N. Balucani, C. Ceccarelli and V. Taquet, 2015, MNRAS, 449, L16–L20

## 16:45 [22] Deuteration of interstellar glycine on low-temperature surfaces: A possible route to the formation of chiral molecules in dense molecular clouds

#### Presenter: Dr. OBA, Yasuhiro

The simplest amino acid glycine (NH\$\_2\$CH\$\_2\$COOH: d\$\_0\$-Gly) is an achiral amino acid. However, if one of the carbon-bound hydrogen is replaced with a deuterium atom, it becomes a chiral molecule (NH\$\_2\$CHDCOOH: d\$\_1\$-Gly). Although there have been no reports on the detection of chiral species in space, chiral glycine has a potential to be one of the primordial chiral molecules in space. We then performed laboratory experiments on the formation of chiral glycine by grain-surface reactions at low temperatures.

Gaseous d\$\_0\$-Gly was codeposited with deuterium (D) atoms or a mixture of hydrogen (H) and D atoms (H:D = 10:1) on an AI substrate (12 K) in an ultra-high vacuum reaction chamber. Reaction products were analyzed by using a high-resolution mass spectrometer.

We confirmed the formation of d\$1\$-Gly and doubly deuterated glycine (NH\$\_2\$CD\$\_2\$COOH: d\$\_2\$-Gly) in the reaction products, even under the H-dominant conditions. This result suggests that the formation of chiral glycine is possible in dense molecular clouds where H atoms dominate over D atoms. The following reactions are considered to play a role for the formation of chiral glycine: (1) NH\$\_2\$CH\$\_2\$COOH + D  $\rightarrow$  NH\$\_2\$CHCOOH + HD, and (2) NH\$\_2\$CHCOOH + D  $\rightarrow$  NH\$\_2\$CHDCOOH. Since reaction (1) has a large barrier, this reaction would not proceed thermally at ~10 K. Quantum-tunneling is therefore necessary for the reaction to proceed at such low temperatures. At the presentation, we will show experimental results in more detail and another pathway to the formation of chiral glycine under the conditions of dense molecular clouds.

#### 17:00 [67] Star formation through the chemical lens: distortions induced and how to avoid them

#### Presenter: Prof. TASSIS, Konstantinos

Observations of star-forming sites rely heavily on the use of molecular tracers. However, the abundance of these tracers is not constant: it is a result of a complex network of chemical reactions, and it depends on the age, density, and dynamical history of the star-forming site. This chemical lens can introduce distortions in our observational understanding of star formation.

In this talk, I will use a suite of chemodynamical models to discuss two such major distorting effects. The first involves measurements of the ratio between mass and magnetic flux in molecular clouds, which determines the relative importance of magnetic and gravitational forces in the evolution of clouds and their cores. When comparing regions with different densities, the effect of depletion of the tracer used (for example OH) can be so severe as to even reverse the direction of the underlying trends: for example, the mass-to-flux ratio may appear to decrease as we move to higher density regions, contrary to theoretical expectations.

The second effect involves the use of neutral/ion pairs to study the processs of ambipolar diffusion (neutral/ion drift) in molecular clouds. The ion and neutral species used in such studies need to be co-spatial at every scale and density if they are to trace the same region, something which, as I will show, is not necessarily the case with the species typically used. I will propose instead new ion-neutral pairs that are good candidates for such observations, because they have similar evolution and are approximately co-spatial

Finally, I will discuss some newly proposed observables with maximal potential for discrimination between different models of cloud evolution and star formation. These results are especially timely as current and future facilities, such as ALMA and SKA, will be able to measure these quantities and contribute to the resolution of long-standing questions in star formation.

#### 17:15 [83] Water and H2O+ in dense galactic nuclei

#### Presenter: Prof. VAN DER TAK, Floris

Dense gas in galactic nuclei is known to feed central starbursts and AGN, but the properties of this gas are poorly known due to the high obscuration by dust. Water and H2O+ are useful to trace the oxygen chemistry of interstellar gas, and its ionization rate.

We present Herschel/HIFI spectra of the H2O 1113 GHz and H2O+ 1115 GHz lines toward 5 nearby prototypical starburst/AGN systems. The beam size of 20" corresponds to resolutions between 0.35 and 7 kpc.

The observed line profiles range from pure absorption (NGC 4945, M82, Arp 220) to P Cygni indicating outflow (NGC 253) and inverse P Cygni indicating infall (Cen A). The profiles of H2O and H2O+ are remarkably similar, indicating that the lines trace the same gas.

We estimate column densities assuming negligible excitation (for absorption features) and using a non-LTE model (for emission features), adopting calculated collision data for H2O and rough estimates for H2O+. Columns range from ~1e13 to ~1e15 cm\$^{-2}\$ for both species, and are similar between absorption and emission components. The H2O/H2O+ ratios are 1.4-5.6, indicating an origin of the lines in diffuse gas. However, the H2O abundance is only ~1e-9, perhaps indicating enhanced photodissociation by UV from the nuclei or depletion of H2O onto dust grains.

We combine our N(H2O+) values with literature data to estimate the cosmic-ray ionization rates for our sample, adopting recent Galactic values for the average cloud density, the atomic hydrogen fraction, and the ionization efficiency. We find zeta\_CR ~1e-16 s\$^{-1}\$, similar to the value for the Galactic disk, but somewhat below that of the Galactic center and well below that of AGN estimates from excited-state H3O+ lines. Since low filling factors appear unlikely, we conclude that the ground-state lines of H2O and H2O+ probe primarily non-nuclear gas in the disks of these centrally active galaxies.

#### 17:30 [72] Molecular cloud formation and dust particle evolution in SILCC simulations

#### Presenter: Dr. PETERS, Thomas

The SILCC project (SImulating the Life-Cycle of molecular Clouds, Walch et al. arXiv:1412.2749;

http://hera.ph1.uni-koeln.de/~silcc/) aims at a more self-consistent understanding of the interstellar medium on small scales and its link to galaxy evolution. We simulate the evolution of the multi-phase ISM in a 500 pc x 500 pc x 10 kpc region of a galactic disc, with a gas surface density of \$\Sigma\_\rm{gas} = 10 M\_\rm{sol}/pc^2\$. The Flash 4.1 simulations currently include an external potential, self-gravity, magnetic fields, heating and radiative cooling, time-dependent chemistry of H\$\_2\$ and CO considering (self-) shielding, and supernova feedback. After summarising the main results of our first generation of simulations and giving an outlook on the latest simulations with additional physics (cosmic ray transport and stellar winds), I will focus on two projects that aim at getting a better understanding of molecular cloud structure (chemical and dynamical): 1) High-resolution simulations of molecular cloud formation out of the diffuse interstellar medium that can be compared with, e.g., observations obtained by the THOR project and 2) Simulations of the Lagrangian evolution of dust particles within the multi-phase ISM, with the long-term aim of producing simulations with a live model of dust properties and opacities that feed back to the chemical and thermodynamical evolution during cloud formation.

#### Poster Viewing - (17:45-18:30)

**Poster Viewing** 

#### Updates on ALMA - (18:30-19:00)

- Presenters: Dr. TESTI, Leonardo

## Tuesday 06 October 2015

## FROM DENSE CORES TO PROTOSTARS (I): Formation of accretion disks, self-gravitating disks, Class 0 sources, outflows, hot cores/corinos - (09:00-12:45)

#### formation of accretion disks, self-gravitating disks, Class 0 sources, outflows, hot cores/corinos

#### time [id] title

#### 09:00 [97] Tracing the chemical evolution of deeply embedded protostars: the ALMA view

Presenter: Dr. JORGENSEN, Jes Kristian

Protostars in their earliest, deeply embedded, stages provide an important astrochemical laboratory, serving as the evolutionary link between dense regions in molecular clouds and the end-products in terms of the emerging protoplanetary disks. In recent years significant progress has been made on understanding the physical and chemical evolution of young stars during through stages. In particular, the Atacama Large Millimeter/submillimeter Array, ALMA, is showing its capabilities for studies of the chemistry of solar-type stars with its high sensitivity for faint lines, high spectral resolution which limits line confusion, and high angular resolution.

In this talk I will discuss the constraints on the chemical structure of deeply embedded protostars offered by recent ALMA observations and some of the important questions emerging. For example, what is the link between the physical and chemical structure of deeply embedded protostars on solar-system scales and how is the chemical evolution of protostars affected by strong (time-dependent) variations in, e.g., the density and temperature during the infall from the parental core to the circumstellar disk?

#### 09:25 [20] Understanding the formation of formamide (NH\$\_2\$CHO), a key precursor of prebiotic chemistry

Presenter: Dr. LOPEZ-SEPULCRE, Ana

One of the major questions regarding the origin of life on Earth is whether the original mechanism that led from simple molecules to life was connected to metabolism or to genetics, both intimately linked in living beings. Formamide (NH\$\_2\$CHO) contains the four most important elements for biological systems, and it has recently been proposed as a precursor of both metabolic and genetic material, suggesting a common chemical origin for the two mechanisms. Moreover, recent experiments have shown that the four nucleobases present in RNA might have naturally formed from formamide during the Late Heavy Bombardment, which further stresses its key role in the synthesis of biogenic molecules.

Formamide was first detected in molecular clouds more than four decades ago. Despite this, dedicated observational studies have started only very recently, as its potential role as a precursor of prebiotic chemistry has become more evident. These studies report the presence of formamide in massive hot molecular cores, one low-mass hot corino, and the comet Hale-Bopp. In the past months, the IRAM Large Program ASAI, dedicated to astrochemical studies of star-forming regions, has revealed new discoveries of NH\$\_2\$CHO in several solar-type protostars and outflow shock spots. The presence of formamide in such a variety of star-forming environments, as well as on a Solar System comet, opens the possibility of an exogenous delivery onto a very young Earth more than 4 billion years ago.

In this talk, we will present the different observational studies of formamide that have been carried out in the past years, with a particular emphasis on our new ASAI results. We will discuss the different chemical pathways that have been recently suggested to explain its formation, which include gas-phase as well as gas-grain reactions, and review the observational constraints brought by ASAI. Finally, we will stress the importance of joining efforts with experts on both theoretical and experimental chemistry in order to make progress. Further dedicated observational studies, particularly with the interferometers ALMA and NOEMA, will be crucial in order to place constraints on the various formation routes so far proposed.

#### 09:50 [4] Astrochemistry at work in pristine protostellar jet-disk systems

#### Presenter: Dr. CODELLA, Claudio

What are the basic chemical mechanisms that led atoms to molecules in star forming regions? What is the role of the pre-solar chemistry in the present chemical composition of the Solar System bodies, planets, comets, and asteroids? The molecular complexity builds up at each step of the process leading to star formation, starting from simple molecules and ending up in Complex Organic Molecules (COMs). The detection of COMs is thus key to understanding the formation of pre-biotic molecules in the interstellar medium and their subsequent delivery onto planetary systems. However, observations of COMs are still instrumental in making progress; it is of paramount importance to have reliable information on the spatial distribution of COMs in order to investigate whether the regions precursor of planetary systems are already rich in COMs and pre-biotic molecules. This requires spatial resolutions less than 100 AU.

We present here ALMA and NOEMA observations at mm and sub-mm wavelengths of Class 0 protostars (such as L1157 and HH212): thanks to the unprecedented combination of high-sensitivities and high-angular resolutions provided by these new interferometers, it is now possible to image in details the earliest stages of a Sun-like star formation. In particular, we show (i) how to disentangle the COMs emission due to different ingredients of the star formation recipe: warm envelopes and cavities opened by hot and fast jets, accretion disks and shocks, and (ii) how to use protostellar shocks as laboratory to investigate the relative importance of the gas phase processes as compared to a direct formation of COMs on the dust grain surfaces.

#### 10:05 [40] Complex organic molecules in Class 0 protostars from the CALYPSO IRAM-PdBI survey

#### Presenter: Dr. BELLOCHE, Arnaud

An increasing number of complex organic molecules have been found in the interstellar medium, in particular in regions where new stars are being formed. While a few of these molecules have recently even been traced back to the prestellar phase in low-mass-star forming regions, the bulk of their emission in the gas phase is detected during the early accretion phase, when the newly-born protostar starts to heat up its envelope, leading to the sublimation of the icy mantles of dust grains. Understanding the chemical processes that lead to the early formation of these complex organic molecules should shed light on the formation of our own solar system, since even more complex molecules have been found in meteorites and comets and may have played a role in the emergence of life on Earth. As part of the CALYPSO -- Continuum And Lines in Young ProtoStellar Objects -- survey with the Plateau de Bure interferometer (http://irfu.cea.fr/Projets/Calypso), we have obtained sensitive, high-angular-resolution (0.4") spectral maps of a large sample of 17 young, low-mass (Class 0) protostars. The survey covers a wide variety of molecular transitions. I will present a census of the complex organic molecules detected in the full CALYPSO sample. The statistical analysis of such a large sample of protostars should help us better understand the formation mechanisms of these molecules and the conditions for the emergence of chemical complexity in the interstellar medium.

#### 10:20 COFFEE BREAK / Poster Viewing / Discussion

#### 11:20 [96] The VLA Nascent Disk And Multiplicity (VANDAM) Survey of Perseus

#### Presenter: Dr. TOBIN, John

The formation of disks and binary systems is thought to begin early in the star formation process. However, there have not been sufficient numbers of young protostars observed with high enough resolution to determine when and where most binaries and disks form. To significantly improve our knowledge of protostellar disks and multiplicity we have carried out the VANDAM survey, a 264 hour Jansky VLA program at wavelengths of 8 mm, 1 cm, 4 cm, and 6 cm toward all known Perseus protostars (N ~ 80) down to 15 AU resolution. The unbiased nature of the survey has enabled us to conduct the most complete characterization of protostellar multiplicity to date, finding evidence for two peaks in the distribution of multiple protostar system separations. Moreover, we have resolved a number of candidate disks toward Class O and I protostars. We have also characterized the free-free jet emission from the protostars and compared it with other outflow diagnostics and the bolometric luminosities. We confirm that the free-free luminosity is correlated with bolometric luminosity, but find evidence for a different power-law relationship depending on the range of luminosities examined. The combined results of this survey demonstrate the power and utility of unbiased surveys toward young stars.

#### 11:45 [37] Sulfur chemistry in Class 0 disks and jets with ALMA

#### Presenter: Dr. PODIO, Linda

While there have been numerous studies of the disk and jet chemistry in evolved T Tauri stars, observations of the jet-disk system in protostars are very difficult due to their embedded nature and to the occurrence of numerous other kinematical components in the circumstellar region (cavities of swept-up material, infalling envelope, static ambient cloud).

I will show how to exploit the combination of the ALMA capabilities and the emission of the sulfur-bearing molecules to simultaneously probe for the first time the forming disk and the jet base in the HH 212 Sun-like protostellar system. SO and SO2 lines turn out to be effective tracers of the collimated and fast molecular jet in the inner few hundreds AU from the protostar. Their abundances indicate that from 1% to 40% of elemental sulfur is converted into SO and SO2 due to shocks in the jet and/or to ambipolar diffusion at the wind base. On the other hand, the SO abundance in the disk is found to be 3 – 4 orders of magnitude larger than in evolved protoplanetary disks around Class II sources. The observed SO enhancement may be produced in the accretion shock at the envelope-disk interface or in the shocks occuring in the disk spirals caused by gravitational instabilities if the disk is partly gravitationally unstable.

#### 12:00 [79] Envelope infall in the youngest protostars

#### Presenter: Dr. STUTZ, Amelia

Protostars and disks are formed within infalling envelopes of molecular gas and dust. The mass infall rate sets many of the conditions for early disk evolution. High infall rates may increase the mass of the protostellar disk enough to force gravitationally instability leading to the formation of binaries or planets and to episodic accretion from the disk to the protostar. Until recently, our ability to directly measure mass infall rates was restricted by severe observational challenges. Today the next generation of interferometers (ALMA and NOEMA) can obtain observations with the required sensitivity and spatial resolution to observe envelope infall on scales down to the expected sizes of protostellar disks (100 AU). With wide-field Spitzer and Herschel surveys of Orion A we have identified a class of protostars, the PACS Bright Red Sources (PBRS) characteristic of the earliest stage (< 25,000 yrs) of Class 0 evolution. Our CARMA observations found compact (~ 2000 AU) envelopes with high column densities. Our more recent NOEMA data exhibit self-absorption profiles in the H2CO line at 225 GHz, precisely measuring infall velocities (at 0.1 kms) down to a spatial resolution of a few hundred 900 AU, approaching the threshold for disk formation. I will discuss our methods for using wide-field IR surveys to find the youngest protostars and our methods for measuring the infall rates in their envelopes. I will discuss what our models of infall and disk formation indicate for our ALMA observations proposed for the current cycle, which are capable of resolving the transition region between the envelope and the protostellar disk. This is the region where the predominantly radial velocities of infall are turned by angular momentum conservation into the rotational velocities of the disk. These observations have the potential to resolve long-standing ambiguities in the interpretation of the protostellar luminosity distribution and our understanding of how the stellar and disk masses are assembled.

#### 12:15 [27] First results from an unbiased ALMA spectral survey of IRAS16293

Presenter: Dr. VAN DER WIEL, Matthijs

The origin and history of prebiotic chemistry in protostars and protoplanetary disks is a main research theme within astrochemistry. With current observational facilities it is becoming possible to routinely detect complex organic molecular species, and also to study their spatial distribution and relative abundances throughout protostellar envelopes and embedded protoplanetary disks. We will show early result highlights from a large ALMA program targeting the binary protostellar system IRAS16293: \*Protostellar Interferometric Line Survey\* (PILS). This data is more than an order of magnitude more sensitive than previous spectral surveys toward this source. In addition, the adopted interferometer configuration allows us to probe spatial scales ranging from \$>\$1000 au down to \$\sim\$35 au. This does not only separate the two binary components very well, it also allows us to resolve protoplanetary disk scales around each of the two components. The combination of high angular resolution, unprecedented sensitivity, and unbiased frequency coverage of an entire atmospheric window provides openings for various investigations. For example, we study the presence and spatial distribution of complex organic molecules around the two sources, chemical fractionation effects of various isotopologues, and dynamical structure of the gas around each source and in between the two components.

#### 12:30 [2] Hydrogen and Nitrogen isotope fractionation in high-mass star forming regions

#### Presenter: Dr. FONTANI, Francesco

The two stable less abundant isotopes of hydrogen and nitrogen, D and 15N, are both enriched in comets and carbonaceous chondrites with respect to the values measured in the proto-solar nebula. This raises the question whether the two enrichments have a common origin, and how both are linked to the past chemical history of the Solar System. I will present new low-angular resolution observations of isotopologues of N2H+ and CN toward dense cores that belong to different evolutionary stages of the massive star-formation process: from massive starless cores, to high-mass protostellar objects, to UC HII regions. These cores represent likely environments similar to that in which our Sun was born, as suggested by recent findings (Ceccarelli et al. 2014, ApJ, 790, L1). Preliminary results indicate (1) a huge spread in the 14N/15N ratio, and (2) a faint anti-correlation between the H/D and 14N/15N ratio. This last result suggests that 15N enrichment is not linked to the parameters that cause D enrichment, in agreement with the prediction by recent chemical models (Roueff et al. 2015, A&A, 576, 99). These models, however, are not able to reproduce the observed large spread in 14N/15N, pointing out that some important routes of nitrogen fractionation could be still missing in the models.

#### FROM DENSE CORES TO PROTOSTARS (II): Hot-core chemistry; laboratory experiments II. Complex organics, PAHs - (14:00-17:45)

#### hot-core chemistry; laboratory experiments II. Complex organics, PAHs

#### time [id] title

#### 14:00 **[77] Deuterium chemistry and nuclear spin conversion on grain surfaces: implication to deuterium enrichment** *Presenter: Prof. WATANABE, Naoki*

Water and some organic molecules were found to be deuterium enriched not only toward various astronomical targets and but also in comets and meteorites. Understanding the formation processes of deuterated species may lead to know how and when those molecules are created. Although gas phase chemistry is certainly important for deuterium enrichment, the role of physicochemical processes on the grain surfaces should be also considered. In fact, the extreme deuterium enrichment of formaldehyde and methanol requires the grain-surface process. In this context, we have performed a series of experiments on the formation of deuterated species of water, formaldehyde, methanol, ethanol, ethane, ethane, methylamine, glycine, and etc. From the results of these experiments and related works, I will discuss the key processes for the deuterium enrichment on grains. In addition, the overview will be presented for the experiments of nuclear spin conversion on grains of which H\$\_{2}\$ is closely related the formation of H\$\_{2}\$

#### 14:25 [99] Chemistry in hot cores: modeling new molecules

#### Presenter: Prof. GARROD, Rob

New molecules continue to be detected in hot cores, and the ALMA telescope is likely to uncover many more over the coming years. Perhaps the most exciting detections involve highly complex molecules with structures that are new to interstellar chemical networks. How can we incorporate these molecules and structures into chemical networks to make sense of new detections?

I will give a brief overview of current approaches to modelling the chemistry of hot cores, and will detail recent efforts to expand the network of grain-surface formation pathways to include newly detected complex species. I will also explore the implications of the new model results, with a view to future observations.

#### 14:50 [43] Formation and recondensation of complex organics during protostellar luminosity outbursts

#### Presenter: Dr. TAQUET, Vianney

During the formation of stars, the accretion of the surrounding material toward the central object is thought to undergo frequent and strong eruptive outbursts, followed by long periods of relative quiescence. Such episodic events have been invoked to resolve the "luminosity problem" whereby the observed luminosity of most low-mass protostars is lower than the accretion luminosity expected from theoretical collapse models (Dunham et al. 2010). The recent detection of a luminosity outburst toward the embedded Class 0 protostar HOPS 383 by Safron et al. (2015) confirms that luminosity outbursts can occur at the earliest stages of star formation when the protostar is still surrounded by a massive envelope. Strong and sudden changes in the protostellar luminosity are consequently thought to influence the chemical evolution in the surrounding envelope.

We investigated the formation and the recondensation of complex organics, including di-methyl ether and methyl formate, during protostellar luminosity outbursts. For this purpose, we updated a gas phase chemical network forming complex organics triggered by the evaporation of interstellar ices. In particular, we updated the rates and branching ratios of electronic recombination reactions, following laboratory experiments, and introduced proton transfer reactions involving ammonia, not included in databases, forming complex organics. It is found that gas phase chemistry is efficient enough to produce COMs with absolute abundances higher than 10\$^{-8}\$ in spite of the short luminosity outburst timescales of a few hundreds years. The low binding energies of the studied COMs relative to water and methanol delays their recondensation and increases their abundance ratios with respect to methanol.

Comparison with observations shows that models assuming constant physical properties are only able to reproduce the observed abundance ratios of a few percents at high methanol abundances. Models predicting the formation of COMs during luminosity outbursts for high density conditions are able to reproduce the abundance ratios higher than 10 % obtained at moderate methanol abundances. Although the current luminosity of most detected embedded protostars would be too low to produce observable hot cores, previous and recent luminosity outburst events would have triggered a formation of COMs in expanded regions with sizes increasing by one order of magnitude.

#### 15:05 [30] Low-temperature hydrogenation and deuteration of solid aromatic hydrocarbon by tunneling

#### Presenter: Dr. HAMA, Tetsuya

Aromatic hydrocarbon is one of the main component of interstellar and circumstellar dust. The hydrogenation and deuteration of interstellar aromatic hydrocarbons is of particular interest for the formation of aliphatic hydrocarbons and their deuterated isotopologues.

Here, we investigated the hydrogenation/deuteration reactions of amorphous solid benzene (C6H6) at low temperatures of 10–50 K. We exposed amorphous C6H6 samples to cold H or D atoms at 120 K. In situ infrared spectroscopy revealed that cyclohexane (C6H12) or deuterated cyclohexane (C6H6D6) are efficiently formed by H or D atom addition. Given the activation barriers and low temperatures, these reactions proceeded via tunnelling.

In addition, we observed only small KIEs. The ratio of the hydrogenation and deuteration rates (H/D) was 1–1.5 at 15–25 K, whereas deuteration by tunneling typically occurs at a rate more than two orders of magnitude smaller than that of the comparable hydrogenation. This indicates that the isotopically insensitive surface processes (e.g., adsorption and diffusion) of the atoms physisorbed on solid C6H6 masked the tunneling KIE, despite tunneling's providing a classically anomalous reaction efficiency.

In comparison to C6H6, polycyclic aromatic hydrocarbons (PAHs) tend to have lower activation barriers to H or D addition owing to the higher flexibility. Therefore, the present results suggest that interstellar PAHs can be hydrogenated or deuterated by the tunneling of H or D atoms at low temperatures, and that the tunneling KIE would not strongly inhibit the deuteration of interstellar aromatic hydrocarbons.

#### 15:20 COFFEE BREAK / Poster Viewing / Discussion

#### 16:20 [60] Laboratory Studies of Molecular Dynamics at the Gas-Solid Interface

#### Presenter: Dr. IOPPOLO, Sergio

My talk will review the most recent laboratory work performed at the Sackler Laboratory for Astrophysics (Leiden University, NL), at the Blake Research Group (Caltech, US), and at the Astrochemistry Group (Open University, UK). Laboratory experiments showed that surface reaction mechanisms on cold interstellar dust grains initiate molecular chemistry through the formation of H2, and likely dominate the formation of complex organic molecules (COMs) in space. For decades, surface complex molecule formation has been thought to be triggered largely by energetic processing. Very recently, my co-workers and I gave the first laboratory evidence that the building blocks of sugars, fats, and proteins can be formed through non-energetic induced surface reactions under dark molecular cloud conditions (Fedoseev et al. 2015). Since the identification of solid complex prebiotic molecules is difficult because of their low expected interstellar abundances and the overlap of their absorption features with those from the more abundant species in the mid-IR, COMs have been only observed in the gas phase in the sub/millimetre range. Novel laboratory THz time-domain techniques combined to THz radiometry have the potential to allow the detection of COMs in the solid phase in the interstellar medium and understand molecular dynamics and desorption mechanisms of complex species by exploring interlayer vibrational and single molecule torsional modes of ices, phonon modes in solids, and the rovibrational transitions of larger gas-phase species at the gas-solid interface.

#### 16:45 [80] The hydrogenation of PAH cations: A journey guided by stability and magic numbers.

Presenter: Ms. CAZAUX, stephanie

The understanding of hydrogen attachment to carbonaceous surfaces is essential

to a wide variety of research fields and technologies such as hydrogen

storage for transportation but also for the formation of cosmic H2 and the identification of stable PAHs in space. For coronene cations as prototypical Polycyclic Aromatic Hydrocarbon (PAH), the existence of magic numbers upon hydrogenation was uncovered experimentally. Quantum chemistry calculations show that hydrogenation follows a site-specific sequence leading to

the appearance of stable cations having 5, 11, or 17 hydrogen atoms attached,

exactly the magic numbers found in the experiments. For these stable closed-shell

cations, further hydrogenation requires appreciable structural changes

associated with a high transition barrier. The occurrence of stable superhydrogenated PAHs is fundamental to identify PAHs in space and assess their

contribution to the formation of H2.

#### 17:00 [14] In-situ particle (re-)acceleration and induced ionisation in protostars

#### Presenter: Dr. PADOVANI, Marco

It is largely accepted that Galactic cosmic rays, which pervade the interstellar medium, originate by means of shock waves in supernova remnants [1]. Cosmic rays activate the rich chemistry that is observed in a molecular cloud [2] and they also regulate its collapse timescale [3], determining the efficiency of star and planet formation, but they cannot penetrate up to the densest part of a molecular cloud, where the formation of stars is expected, because of energy loss processes and magnetic field deflections [4,5,6,7]. Recently, observations towards young protostellar systems showed a surprisingly high value of the ionisation rate [8,9], the main indicator of the presence of cosmic rays in molecular cloud. Synchrotron emission, the typical feature of relativistic electrons, has been also detected towards the bow shock of a T Tauri star [10]. Nevertheless, the origin of these signatures peculiar to accelerated particles is still puzzling. \*Here we show that particle acceleration can be driven by shock waves occurring in protostars.\* We found that shocks in protostellar jets can be strong accelerators of protons, which can be easily boosted up to relativistic energies. Another possible efficient acceleration site is located at the protostellar surface, where shocks caused by impacting material during the collapse phase are strong enough to accelerate protons. While electron acceleration is not efficient because of Coulomb losses, secondary electrons created during the ionisation process can reach relativistic energies. \*Our results demonstrate the possibility of accelerating particles during the early phase of a proto-Solar-like system and can be used as the argument to support available observations.\* The existence of an internal source of energetic particles can have a strong and unforeseen impact over the stellar and planet formation process as well as on the formation of pre-biotic molecules.

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#### 17:15 [56] Understanding the formation of astrobiological molecules in star-forming regions

Presenter: Dr. RIVILLA, Victor Manuel

The increasing number of detections of complex organic molecules around young stellar objects strongly suggests that they are part of the material of which planetary systems are made of. These molecules play a central role in interstellar prebiotic chemistry and may be directly linked to the origin of life. Since the hot and dense molecular cores surrounding massive stars harbor the richest chemistry in the insterstellar medium, they are the best natural laboratories to study the formation of these complex molecules. While the detection of the simplest amino acids such as glycine still remains elusive, the search of two other families of prebiotic molecules has been more successful: aldoses and polyols. The monosaccharide sugar \*\*glycolaldehyde\*\*, \*\*CH2OHCHO\*\*, is the simplest representative of the aldoses. This molecule can react with propenal to form ribose, a central constituent of RNA. The simplest representative of the polyols is the reduced alcohol of glycolaldehyde, \*\*ethylene glycol\*\*, \*\*(CH2OH)2\*\*. In my talk I will present our results from observations towards the hot molecular core G31.41+0.31, one of the most chemically rich astronomical sources. Among many other simpler molecules, we have confirmed the presence of glycolaldehyde (for the first time outside the center of our galaxy) and ethylene glycol, along with their proposed precursor, the \*\*formyl radical HCO\*\*. I will discuss how these findings can help us to understand the formation of these building blocks of life in the insterstellar medium, with the help of chemical models and laboratory works.

#### 17:30 [47] Chirped Pulse Techniques Applied to Astrochemistry and the Search for PAHs

Presenters: Dr. STEBER, Amanda, Mr. ARENAS, Ben

Radio astronomy has been an important method for identification of molecular constituents in the interstellar medium (ISM). One way to do this is by matching microwave and millimeter wave laboratory spectra to those obtained by radio observatories. Until now, the availability of laboratory data has been sufficient to keep up with the influx of astronomical data. However, with new and upgraded observatories, such as the Atacama Large Millimeter Array (ALMA), coming online that is about to change. Because of this, a move towards revolutionizing microwave and millimeter wave techniques has come about. In this laboratory, we aim to upgrade existing chirped pulse microwave techniques to take advantage of these advances, in order to increase the throughput of astronomically relevant data in this lab. We also plan to use discharge methods in order to begin investigating a top down approach, in which we look at the fragments that form when we take large complex molecules and subject them to the discharge.

#### Poster Viewing: Poster Viewing - (17:45-18:30)

**Poster Viewing** 

#### SOFIA and IR Astrophysics - (18:30-19:00)

- Presenters: Prof. ZINNECKER, Hans

## Wednesday 07 October 2015

## FROM PROTOSTARS TO PROTOPLANETARY DISKS (I): Class I sources, Class II sources, disks around Herbig Ae stars, disks around Brown Dwarfs - (09:00-12:45)

Class I sources, Class II sources, disks around Herbig Ae stars, disks around Brown Dwarfs

time [id] title

09:00	[94] The Physics and Chemistry of Gas Rich Disks from Young to Old
	Presenter: Prof. BERGIN, Edwin
	In this talk I will review our current, and evolving, understanding of the
	physics and chemistry of gas rich disks, including the youngest stages as
	the disk is forming. The record of the earliest stages of disk formation is only now
	being constrained and it is an
	open question as how much of the initial chemical composition is altered during
	this stage. In this light, I will discuss key aspects of this stage including the
	variability of accretion and the potential for disk formation to alter the composition inherited
	from the cold quiescent pre-stellar phase.
	At the Class II stage, disks are exposed to both stellar and interstellar UV/X-ray radiation along the
	the potential presence of galactic cosmic rays, which
	heats disk surfaces, provides ionizing agents to power chemical reactions, and links the
	neutrals to magnetic fields. We will summarize what is known about the propagation of these agents, including a discussio
	of the penetration of galactic cosmic rays.
	The resulting chemistry is dominated by the formation of simple species for which we now
	have a host observational constraints from spatially unresolved data and a growing body of resolved detections from ground-based interferometers. Thus, we will discuss how observations of simple species
	are potentially revealing dominant effects in the overall chemistry, while potentially setting limits on the formation of
	complex organics.
	As astrochemists we aim to explore the chemical composition associated with planet formation.
	In the current age of ALMA we must now begin to link our astronomical understanding
	to that of the record the solar system and beyond. Thus, where possible, I will discuss potential links
	to the our knowledge regarding the formation and chemistry of small and large bodies in the
	solar system along with giant planets in other planetary systems.
)9:25	
	[92] Evolution of Solids The Missing Link
	Presenter: Dr. BIRNSTIEL, Til
	The evolution of solids in circumstellar disks is governed by transport processes and collisional growth. These processes
	are in turn driven by the dynamics of the gas disk. Dust evolution is therefore not only the first step towards forming
	planets, it is also a powerful probe of the structure and dynamics of the gas disk.

Furthermore, key volatiles such as water or CO form/freeze-out on the surfaces of grains. Many aspects of the chemical evolution of disks thus depend on the evolution of solids because particles efficiently migrate inward towards the star. Solids can therefore act as a conveyor belt for frozen-out volatiles. This mode of transport easily dominates other transport processes, such as diffusion or meridional flows.

Upcoming radio interferometers and high contrast imaging will soon deliver a wealth of observations of unprecedented resolution and sensitivity. To make use of the observed dust continuum and molecular line emission, the processes that drive the evolution of solids will have to be well understood. In this talk, I will review recent advances in theoretical modeling, their impact on disk chemistry, and how recent observations already foreshadow an exciting future of the field of planet formation and its chemistry.

#### 09:50 [8] Disk mass determination through CO isotopologues

#### Presenter: Mrs. MIOTELLO, Anna

One of the key properties for understanding how disks evolve to planetary systems is their overall mass, combined with their surface density distribution.

So far, virtually all disk mass determinations are based on observations of the millimeter continuum dust emission. To derive the total gas + dust disk mass from these data involves however several big assumptions. The alternative method is to directly derive the gas mass through the detection of carbon monoxide (CO) and its less abundant isotopologues. CO chemistry is well studied and easily implemented in chemical models, exception made for isotope-selective processes.

For the first time CO isotope-selective photodissociation was implemented in a full physical-chemical code (Miotello et al., 2014). The main result is that if isotope-selective effects are not considered for the data analysis, disk masses can be underestimated by an order of magnitude or more. For example, the mass discrepancy found for the renowned TW Hya disk may be mitigated by this implementation. We show that if CO isotope-selective photodissociation is implemented and if atomic carbon (C) is depleted by a factor of 10, the puzzle of TW Hya disk mass is solved (Miotello et al., in prep.). Moreover, mass correction factors are derived and provided for different disk properties in order to account for isotope-selective effects (Miotello et al., in prep.).

#### 10:05 [18] Compact SO Emission around Protostars: A Possible Ring due to Accretion Shocks?

#### Presenter: Prof. OHASHI, Nagayoshi

We report compact SO emission around three class 0/I protostars found as byproducts during the ALMA observations searching for Keplerian disks. The three protostars are L1527 IRS, TMC1A, and L1489 IRS in Taurus. The ALMA observations have found Keplerian disks of 50-700 AU in radius around them in C\$^{18}\$O (\$2-1\$) emission, and also have revealed that the materials surrounding the disks are accreting to them, suggesting that these disks are still under formation. In addition to C\$^{18}O (\$2-1\$) emission tracing the Keplerian disks and the surrounding infalling materials, compact SO(6\$ 5-5 4\$) emission is found. The size of the SO emission is ~200-600 AU, much more compact compared to the C\$^{18}O emission. The SO emission also exhibits rotating motions with the same directions as those of the Keplerian rotation. The rotation patterns of the SO emission are, however, very different from those of the Keplerian disks, i.e., although Keplerian rotation shows clear spin-up motions, the SO emission shows rigid-body-like rotation. The most possible origin of the compact SO emission with rigid-body-like rotation is a ring rotating around the protostar. We consider that SO molecular abundance is locally enhanced in a ring region around the protostar because of higher dust temperatures (40-60 K) caused by the accretion shock. A simple 1-D shock model shows that SO sublimation is possible with relatively low pre-shock velocities ( $\sim 2 \text{ km s}^{-1}$ ) and high pre-shock density ( $\sim 10$ , 9, cm,  $^{-3}$ ), and that the heated layer is rather narrow because of the short cooling timescale. In the case of L1527 IRS, LVG analysis using three different transitions of SO observed by ALMA has been performed to investigate the physical conditions of the SO emission region. The analysis suggests that the kinetic temperature of the SO gas is most likely ~ 30 K, which is not as high as the sublimation temperature of SO (40-60 K). This suggests that the SO ring has a thin postshock layer with a higher temperature at its outermost radius, while the SO recondenses onto grain surfaces at the inner edge of the ring.

#### 10:20 COFFEE BREAK / Poster Viewing / Discussion

#### 11:20 [1] Modeling Complex Organic Molecules Formation in Cold Cores

#### Presenter: Dr. CHANG, Qiang

The recent discovery of terrestrial-type complex organic molecules(COMs) in astronomical sources that are as cold as 10 K challenges current COMs formation astrochemical models because COMs were thought to be formed by combination of diffusive radicals on dust grain surfaces, however, radicals can hardly diffuse at 10 K. Moreover, the abundance of some COMs are found to be strongly correlated. In this talk, we investigate a scenario in which non-diffusive chemistry is important for both COMs and their precursor formation. Our simulations are performed by the recently developed unified macroscopic--microscopic Monte Carlo approach. Reactive desorprion mechanism is also included to desorb COMs from grain surface. The observed abundances of a variety of organic molecules in cold cores can be reproduced in our models. The strong

correlation between the abundances of methyl formate and dimethyl ether in cold cores can also be explained.

#### 11:45 [21] DCO\$^{+}\$: tracer of X-ray ionization in the inner warm disk surface

#### Presenter: Dr. FAVRE, Cecile

Determination of the D/H ratios is valuable for understanding the chemical and physical conditions at earlier phases of protoplanetary disks formation, in which planets formation may occur. Understanding deuterium fractionation is thus key to explain the D/H distribution pattern found in the various bodies of our solar system. To investigate the different key gas-phase deuteration pathways that can lead to the formation of DCO\$^{+}\$, we have modeled the chemistry of DCO\$^{+}\$ in protoplanetary disk [1]. I will present some of these results. In particular, our modeling shows that the recent update in the exothermicity of the reaction involving CH2D\$^{+}\$ as a parent molecule of DCO\$^{+}\$ favors deuterium fractionation in warmer conditions (T \$\ge\$ 50 K) [2]. Our analysis shows that the formation of DCO\$^{+}\$ is enhanced in the inner warm surface layers of the disk where X-ray ionization occurs. Our findings suggest that DCO\$^{+}\$ is a tracer of X-ray ionization of the inner disk but not of the CO snow-line.

[1] Favre et al. (2015), The Astrophysical Journal Letters, 802, L23

[2] Roueff et al. (2013), Journal of Physical Chemistry A, 117, 9959

#### 12:00 [55] Accretion disks in young high-mass stars

#### Presenter: Dr. BELTRAN, Maite

Spatially resolved molecular line observations have revealed circumstellar disks in Keplerian rotation around young stellar objects with masses up to 30 \$M\_\odot\$. Line emission observations have been crucial in identifying and characterizing these disks and have allowed us to study their dynamics. In this contribution, I will discuss their properties and evolution and compare them to the circumstellar structures around lower mass counterparts. Particularly, I will discuss the mass accretion of disks as a function of stellar mass and time to get insights into the universality of star-formation models.

#### 12:15 [36] Complex Organic Nests of Low-Mass Protostars

#### Presenter: Ms. DROZDOVSKAYA, Maria

Complex organic molecules are fused with low-mass star-forming systems. Such species have been observed on- and off-source in hot and cold environments, respectively [e.g., 1, 4, 5]. During the formation of the star-disk system these compounds can potentially contaminate protoplanetary and proto-cometary materials with organics. In this talk, physicochemical models are presented, including wavelength-dependent radiative transfer and an extensive gas-grain chemical network. Model results on the effects of dynamic infall from the prestellar core towards the protoplanetary disk will be discussed. A dedicated set of model results will be shown for the midplanes of disks and the ice content therein, which is expected to trace the dominant portion of the volatile material for the larger forming solid bodies. The results of our dynamical model are contrasted by the outcomes of a static model [3]. Also, the distribution of complex organics themselves, i.e., trace species of the icy mantles, will be shown. Finally, the off-source distribution of complex organics is investigated by means of a static model on much larger scales of several thousand AU. The results show that the cavity walls illuminate in a time-dependent and species-variant fashion. In addition, a complex organic ice-rich torus in the inner envelope encompassing the young low-mass protostar appears in the simulations, which is not reflected in the gas phase. Furthermore, complex organics are demonstrated to have unique lifetimes and be grouped into early (formaldehyde, ketene, methanol, formic acid, methyl formate, acetic acid, glycolaldehyde) and late (acetaldehyde, dimethyl ether, ethanol) species [2].

[1] Arce H. G., Santiago-Garc all J., Jørgensen J. K., Tafalla M., Bachiller R., 2008, ApJ, 681, L21

[2] Drozdovskaya M. N., Walsh C., Visser R., Harsono D., van Dishoeck E. F., 2015, MNRAS, in press [3] Drozdovskaya M. N. et al., 2015, in prep.

[4] Öberg K. I., Bottinelli S., Jørgensen J. K., van Dishoeck E. F., 2010, ApJ, 716, 825

[5] Öberg K. I., van der Marel N., Kristensen L. E., van Dishoeck E. F., 2011, ApJ, 740, 14

## 12:30 [25] Kinematics of an Accretion Disk in a Proto-Brown Dwarf Candidate, L328-IRS, and Its Implication *Presenter: Dr. LEE, Chang Won*

L328-IRS is one of the Very Low Luminosity Objects exhibiting typical properties of a protostar, but, the luminosity (\$\sim 0.05 \lsun\$) far below than expected from the least massive protostar by the standard star formation theory. This was found to derive an bipolar outflow in the sub-parsec scale outflow. The mass accretion rate (\$\sim 3.6\times 10^{-7} \\msun\$/yr ) inferred from the bipolar outflow is an order of magnitude less than the canonical value for a protostar. This may suggest that L328-IRS will accrete the mass of a brown dwarf, but not that of a star during the typical period of a protostar. Given that its envelope mass is small (\$\sim 0.09 \msun\$ ) and 100\% star formation rate is unlikely, it is suggested that L328-IRS is likely a proto-brown dwarf. Inward motions are found in global scale in the L328 cloud and its sub-cores. L328 is fairly well isolated from other nearby clouds and seems to be forming three sub-cores simultaneously through a gravitational fragmentation process. Altogether, these all leave L328-IRS as one of the best examples for studying the formation processes of the brown dwarf.

In our poster we will focus on our recent ALMA data for this source, especially on the first discovery of a rotating disk in this proto-brown dwarf.

Our preliminary results on its kinematics is surprising in the sense that it is neither Keplerian nor in a mode of angular momentum conservation.

The rotation velocity decreases toward the center of the disk, L328-IRS, in a rather similar pattern to that of solid disk rotation,

but with a faster speed in the inner region than expected from the purely solid disk rotation.

Why the dynamics of the disk of L328-IRS is different from the one for typical protostars and what would be an important implication of this result will be discussed in the poster.

#### FROM PROTOSTARS TO PROTOPLANETARY DISKS (II): Protoplanetary disk chemistry; laboratory experiments III. Surface chemistry and dust evolution - (14:00-17:45)

protoplanetary disk chemistry; laboratory experiments III. Surface chemistry and dust evolution

time [id] title

#### 14:00 [98] Chemical evolution along the journey from protostar to protoplanetary disk

Presenter: Dr. WALSH, Catherine

I will review recent advances in observations, models, and the laboratory, which have shed new light on the chemical evolution as a protostar evolves to form the protoplanetary disk. ALMA 'Early Science' observations have allowed an unprecedented view of the molecular gas in protostars and disks on size scales approaching those of the inner Solar System (< 50 AU). In conjunction, 'hot off the press' results from the Rosetta mission have thrown open the doors regarding the origin of molecular material in disks, and its subsequent accumulation into planetesimals. Furthermore, laboratory efforts on the quantification of chemical processes thought to be important for building chemical complexity, are providing vital clues on the origin of complex organic molecules across the spectrum of astrophysical sources in which they are detected. It is truly an exciting era for astrochemistry. I will finish by discussing how these cutting-edge observations and laboratory data are providing a stimulating challenge for modellers.

#### 14:25 [102] Non-energetic processes at the surface of dust grains

#### Presenter: Prof. DULIEU, Francois

The synthesis of molecules is a long and convoluted process. The molecular universe begins at the border of molecular clouds, and chemical complexity increases throughout the star formation process (Caselli & Ceccarelli 2012). Interstellar dust grains play many roles in the evolution of clouds, stars and planets, and among them, grains are effective catalytic centers, sometimes called chemical nanofactories. Unfortunately the direct observation of the chemical solid phase is a challenge for astronomy, and therefore a very good knowledge of the processes between gas and grains is required to handle gas phase observables.

For a decade we have developed laboratory astrophysics experiments centered around the synthesis of molecules from atoms and radicals on cold amorphous surfaces, mimicking interstellar conditions (Dulieu et al 2005). In my presentation I will explain how in the lab we can study some of the chemical networks, thanks to the example of the formation of water (Chaabouni et al 2012). I will briefly present new advances in chemistry, and focus on potentially meaningful mechanisms. I will explain how newly formed in the gas phase after their formation on the surface, and try to estimate the efficiency of this chemical desorption (Dulieu et al 2013, Minissale et al 2015a). I will finish by presenting new results about binding energies of O, and N atoms (Minissale et al 2015b), and some new aspects of the segregation of the species at the surface of grains that can affect their desorption energies (Noble et al 2012, 2015).

- Paola Caselli and Cecilia Ceccarelli. 2012. « Our Astrochemical Heritage ». The Astronomy and Astrophysics Review 20 : 1■68. doi:10.1007/s00159-012-0056-x.

 Francois Dulieu, Emanuele Congiu, Jennifer Noble, Saoud Baouche, Henda Chaabouni, Audrey Moudens, Marco Minissale, et Stéphanie Cazaux. 2013. « How micron-sized dust particles determine the chemistry of our Universe ».
 Nature Scientific Reports 3 : 1338. doi:10.1038/srep01338.

- Marco Minissale, Francois Dulieu, Seyit Hocuk, Stephanie Cazaux, "Last gas before the frost: part I Quantifying chemical desorption and its impact on interstellar gas", submitted to A&A

- Marco Minissale, Emanuele Congiu and Francois Dulieu, "Direct measurement of desorption and diffusion energies of O and N atoms physisorbed on amorphous surfaces" submitted to A&A

- Noble, J. A., Congiu, E., Dulieu, F., & Fraser, H. J. (2012). "Thermal desorption characteristics of CO, O2 and CO2 on non-porous water, crystalline water and silicate surfaces at submonolayer and multilayer coverages ". Monthly Notices of the Royal Astronomical Society, 421(1), 768–779. doi:10.1111/j.1365-2966.2011.20351.x

- Jenny Noble, Stephan Diana and Francois Dulieu, "Segregation of O2 and CO on the surface of dust grains determines the desorption energy of O2", accepted in MNRAS

#### 14:50 [13] Deuterium and 15-N fractionation in protoplanetary disks

Presenter: Prof. ÖBERG, Karin

Isotopic fractionation patterns is a popular tool to date Solar System and interstellar material. Nitrogen and hydrogen fractionation, i.e. the enhancement of deuterium and \$^{15}\$N in molecules, are both expected to be efficient at the low temperatures found in pre-stellar cores an protoplanetary disk midplanes. These enhancements can survive the warmer phases of star and planet formation, maintaining a record of the environment where the molecules first formed. In ALMA Cycle 2, we carried out a survey of deuterated molecules in protoplanetary disks with the aim to establish a direct link between interstellar and Solar System deuterium fractionation. In addition to spatially resolving the distributions of several deuterated molecules and their non-deuterated analogs, we also detected \$^{15}\$N-bearing molecules in disks for the first time. I will present the results of this survey and the constraints it places on the deuterium and nitrogen fractionation chemistry in protoplanetary disks. Highlights include the discovery of a spectacular DCO\$^+\$ double-ring around the T Tauri star IM Lup, and of cometary \$^{15}N/\$^14}N ratios in HCN in the disk around MWC 480.

#### 15:05 [24] T Tauri disk gas masses measured from hydrogen deuteride

Presenter: Dr. MCCLURE, Melissa

The total gas mass of a protoplanetary disk is a fundamental, but poorly determined, quantity. A new technique (Bergin et al. 2013) has been demonstrated to assess directly the bulk molecular gas reservoir of molecular hydrogen using the HD J=1-0 line at 112 microns. In this work we present a survey of T Tauri disk observations of the HD line. Line emission is detected in two cases at >3 sigma significance. Using detailed disk structure models, including the effect of UV gas heating, we determine the amount of gas required to fit the HD line and the amount of dust required to fit the observed disk spectral energy distributions. For both disks, the amount of gas required is more than the MMSN value, and the gas/dust ratio within the millimeter dust outer radius is at least a factor of two lower than that of the ISM. We discuss the implication of this result for these disks' chemistry and the disk mass probability distribution.

15:20 COFFEE BREAK / Poster Viewing / Discussion

#### 16:20 [117] The characteristic of dust in molecular clouds

#### Presenter: JÄGER, Cornelia

In the interstellar medium (ISM), amorphous silicates and carbonaceous materials must be the result of grain condensation and growth at low temperatures and densities in molecular clouds. In our laboratory, we have designed experiments to study the cold condensation and processing of silicates and carbon material in the ISM. Molecular precursors that are the results of destructive dust processes in the ISM were produced in the laboratory and deposited on substrates kept at temperatures between 6 and 20 K. We have studied the condensation of refractory siliceous and carbonaceous dust. Our experimental results support the hypothesis that interstellar silicates and carbon are formed by accretion through barrierless reactions. In addition, first results on the co-accretion of carbonaceous and silicate species in ices and the formation of mixed dust will be discussed. After the reformation of dust in molecular clouds, the refractory material is continuously processed by ion bombardment resulting in a ceaseless change of the dust composition and structure.

### 16:45 [33] The role of fundamental surface processes on astrochemistry: a computational chemistry perspective

#### Presenter: Dr. CUPPEN, Herma

The formation of many saturated species that have been observed in a wide variety of astronomical objects cannot be explained by gas phase chemistry alone and it is clear that surface chemistry must play a crucial role. Most of this chemistry occurs through a diffusive mechanism. Gas-grain models which include this type of chemistry, use however many assumptions on input parameters such as diffusion rates and on the structure of the ice mantle.

I will show how computational chemistry tools can help to get more information on fundamental surface processes such as diffusion and energy dissipation. This information can serve as input for astrochemical models. I will show how these processes impact not only on the surface chemistry but also on thermal and non-thermal desorption rate, such as reactive desorption. Non-thermal desorption is often envoked to explain observed gas phase abundances in cold regions. I will focus on simple molecular species, like CO, H\$\_2\$O, CH\$\_4\$, and CO\$\_2\$, but I aim to make it more general to obtain predictive power for more complex species.

#### 17:00 [81] Impact of dust opacities and disk shape on the physio-chemical state of protoplanetary disks

Presenter: Dr. WOITKE, Peter

The internal physical and chemical structure of protoplanetary disks is of fundamental importance to understand how planets form. To infer this structure from observations, new 'holistic' disk models have been developed in the frame of the EU FP7 project \*DIANA\* which include detailed 2D dust and PAH radiative transfer, thermo-chemical gas and ice modeling, and 3D diagnostic radiative transfer to consistently predict all line and continuum observations, from optical to centimeter wavelengths, based on a single model.

The dust size, opacity and disc shape parameters are found to have a strong impact on the computed temperature and chemical structure of protoplanetary disks, and hence on the predicted continuum and line observations. More evolved dust properties (larger grains) and stronger dust settling are generally found to amplify gas emission lines at optical to far-IR wavelengths, because the heating UV radiation can penetrate deeper into the disk gas in these cases.

We are proposing new dust opacities for protoplanetary disk models, which account for the properties of evolved dust, and discuss how multi-wavelength line and continuum observations can be used to infer the physio-chemical structure of protoplanetary disks.

#### 17:15 [59] Tracing the evolution of the nitrogen isotopic composition around protostars

#### Presenter: Dr. WAMPFLER, Susanne

The volatile elements hydrogen, nitrogen, and oxygen show large isotopic variations among the solar system bodies. These isotopic heterogeneities are peculiar, because the isotopic composition of solar system matter is generally quite homogeneous. Thus, understanding the origin of the volatile stable isotope anomalies will contribute substantially to our understanding when and where the different solar system materials formed.

The Genesis space mission has demonstrated that the solar system solids and the gas reservoir do not share a common nitrogen isotopic composition. The terrestrial planets, comets, and meteorites are significantly enriched in rare  ${}^{15}N$  compared to the Sun and the gas giants. Two processes have been proposed to explain these variations in the  ${}^{14}N/{14}N/{15}N$  ratio: low-temperature chemical fractionation and isotope-selective photochemistry. However, the relative importance of the two processes is still unclear.

Measurements of the \${}^{14}\$N/\${}^{15}\$N ratio in prestellar cores and protostars can be used to tackle the question what mechanism controls the nitrogen isotope composition during the star formation process. However, such measurements are challenging because of the low abundance of \${}^{15}\$N-bearing isotopologues. Thanks to new broad bandwidth receivers at single-dish telescopes and interferometers with unprecedented sensitivity, more comprehensive isotopic studies of star-forming regions can now be carried out.

Different spatial signatures are expected from the chemical fractionation and photochemistry scenarios. Therefore, spatially resolved measurements of the \${}^{14}\$N/\${}^15}\$N ratio are key to probe these spatial variations and constrain the dominant fractionation mechanism. We will present the first spatially resolved measurement of the \${}^{14}\$N/\${}^15}\$N ratio around the Class 0 protostar NGC 1333 IRAS 2A with the IRAM Plateau de Bure Interferometer. Early results from high-resolution observations of the young stellar object IRAS 16293-2422 with ALMA can also be expected. In addition, we will present the results from our nitrogen isotope studies of a protostar sample with different single-dish telescopes.

ALMA now offers the possibility to measure isotopic ratios even in protoplanetary disks, so that in the near future we will be able to trace the evolution of the \${}^{14}\$N/\${}^15}\$N ratio during protostellar evolution and address the origin of the solar system's nitrogen isotope anomaly.

#### 17:30 [17] Resolved High-J 13CO Emission as a Sensitive Probe of Disk Structure and Chemistry

Presenter: Ms. SCHWARZ, Kamber

We present our new ALMA observations of \$^{13}\$CO and C\$^{18}\$O 6-5 in TW Hya. These data include the first direct detection of the CO snow line in this system and exciting evidence of non-Keplarian structure in the inner 20 AU. Snow lines represent volatile sublimation fronts in protoplanetary disks, which are believed to aid in the growth of planetesimals. In this regard the \$^{13}\$CO 6-5 image shows a precipitous drop at 25 AU. Based on detailed models, and the previous detection using N\$\_2\$H\$^+\$ (Qi et al 2013), this drop is constant with the evaporation front. We will also show that these data provide glimpses of structure in the radial abundance of CO, which has been shown to be depleted in this source. Additionally, these observations clearly show strong high velocity emission in the inner disk. Our modeling of these spectra indicate that a simple Keplerian velocity field is incapable of reproducing the observed line profiles, consistent with other recent high resolution observations of protoplanetary disks (e.g. Rosenfeld et al. 2013, Casassus et al. 2015). Using Markov Chain Monte Carlo techniques we explore a range of modified disk models, including a disk with a warped inclination and deviations from Keplerian rotation induced by an embedded planet. In all, this work provides the first complete picture of the CO abundance in an evolved T Tauri disk and shows the utility of high J CO emission as a tracer of structure likely induced by hidden young planets.

#### Poster Viewing: Poster Viewing - (17:45-18:30)

#### **Poster Viewing**

#### Commemorating Alex Dalgarno - (18:30-19:00)

- Presenters: Prof. VAN DISHOECK, Ewine

## Thursday 08 October 2015

### PROTOPLANETARY DISK EVOLUTION AND SOLAR SYSTEM (I): Transient disks, debris disks - (09:00-12:30)

#### transient disks, debris disks

#### time [id] title

#### 09:00 [90] The role of ice lines in planet formation

Presenter: Dr. JOHANSEN, Anders

I will discuss new results on the formation of planets and the role of ice lines in planet formation. Pebbles play a crucial role both for the formation of planetesimals by particle concentration followed by gravitational collapse and for the subsequent rapid growth of planets by pebble accretion. The chemical composition of the pebbles depends strongly on the local temperature of the protoplanetary disc. Near ice lines, diffusion of vapour leads to efficient pebble growth. These large pebbles can trigger planetesimal formation, so that planetary seeds start to grow outside ice lines. I will show that the current location and mass of Jupiter are consistent with formation near the CO ice line.

#### 09:25 [109] Constrains on structure and composition of the inner regions of transitional Herbig Ae star disks

Presenter: DOMINIK, Carsten

Transitional disks are protoplanetary disks with large inner holes, large enough to cause a significant drop in the SED. It has recently been shown that most if not all of the sample of isolated Herbig Ae stars have clear indications for the existence of such holes. Interestingly, most of these objects still have host dust near the sublimation zone. I will discuss mechanisms for the creation of such structures, and I will evaluate constrains on the composition and structure of these regions.

#### 09:50 [12] Chemical footprint of a nascent planet

Presenter: Dr. FUENTE, Asunción

The formation of planetesimals requires that primordial dust grains grow from micron- to km-sized bodies. As dust grains grow, they start to decouple from the gas and drift radially towards the central star. Therefore, planetesimal formation has to happen in time-scales shorter than radial drift. One way to halt the inward drift is by developing a local maximum in the radial surface density of the gas that would act as a dust trap. Dust traps have been identified in transitional disks using the dust continuum emission at longer wavelengths (mm). However their detection remains difficult in molecular lines. Our data show the chemical footprint of the presence of a dust trap in a transitional disk. Sulfur monoxide has been imaged in the transitional disk around the Herbig Ae star, AB Auriga. This species presents an odd spatial distribution with a hole towards the dust trap. This hole is the consequence of the enhanced gas densities within the trap and it is so far the best example of how the gas dynamics, the grain growth and the gas chemistry are coupled. Hydrodynamical simulations couple to a time-dependent chemical model are able to explain the observed trend and prove that the sulphur chemistry can be used as a tool to investigate the planet formation process. SO is the second S-bearing molecule detected in a PPD (the first was CS) and opens the possibility to study the sulphur chemistry in a proto-solar nebula analog. Besides the high level of sulfur in the Sun (S/Si \$\sim\$0.5), sulfur is widespread in the Earth, the Venusian atmosphere, in the Martian regolith, it is present in Jupiter and Saturn, and is specially abundant in Io. The comprehension of the sulfur chemistry is of paramount importance to understand the formation of our own planetary system.

#### 10:05 [31] How small are the smallest dust grains in debris discs and why?

Presenter: Ms. PAWELLEK, Nicole

The minimum size of dust grains in debris discs is a sensitive indicator of a variety of physical processes operating in these systems. We analysed a sample of 32 Herschel-resolved debris discs to derive the minimum grain size and found an intriguing trend of that size changing with the luminosity of the debris disc host star. The trend is statistically significant and is pretty robust against variations of the assumed dust chemical composition and porosity. The effect goes beyond a simple explanation that grains around more luminous stars have to be larger in order not to be blown out by the stronger radiation pressure of such stars. Instead, we show that the trend can be related to the microphysics of collisions that replenish the visible dust.

Alternatively or additionally, the trend can be explained by assuming that debris discs of more luminous stars have higher dynamical excitations than those of less luminous primaries. If true, this would imply that the protoplanetary progenitors of debris discs around the stars of earlier spectral types were more successful in producing massive stirrers, be it big planetesimals of planets. As a by-product of our analysis, we suggest a recipe of how to estimate the true radii of spatially unresolved debris discs, based solely on their spectral energy distribution.

10:20 COFFEE BREAK / Poster Viewing / Discussion

#### 11:20 [100] Origin, evolution and frequency of gas in debris disks

#### Presenter: Dr. WYATT, Mark

A growing number of main sequence stars show evidence for circumstellar gas. It is most often CO that is detected, which is puzzling because this molecule should have a short lifetime due to photo-dissocation by the interstellar radiation field. Since this gas is usually found around young stars, the most obvious explanation would be that this is a remnant of the primordial protoplanetary disk that provides key clues about disk dispersal processes. However, in the case of beta Pictoris there is strong evidence from the disk morphology that the gas is secondary, i.e., produced in the destruction of icy planetesimals. To interpret these observations, and to model how the gas evolves, it has been necessary to develop new models, because the low optical depth of debris disk environments and non-standard gas composition invalidates the assumptions used in protoplanetary disk modelling. This talk will review our understanding of gas in debris disks, starting with the frequency with which main sequence stars show evidence for gas. We will present new ALMA observations of CO in the beta Pic disk that map its distribution and provide valuable information on the physical conditions in this disk. We will also discuss a new model for the origin and evolution of gas in debris disks that includes the evolution of the photo-dissociation products that can be constrained observationally.

#### 11:45 [32] Collisional modelling of the AU Mic debris disc

#### Presenter: Mr. SCHÜPPLER, Christian

Being remnants of the planet formation process, debris discs consist of (invisible) planetesimals and collisionally-replenished dust. Observations from optical to submm wavelengths reveal their presence around at least 20% of main-sequence stars. Systems that are spatially resolved at multiple wavelengths and have densely sampled SEDs allow us to more tightly constrain the physical properties of debris discs. We performed an in-depth collisional modelling of the prominent debris disc around the young M star AU Mic, aiming at a comprehensive understanding of the dust production and the dynamics of the disc objects in this system. The simulations started from a distribution of planetesimals and followed the production and loss of material in a collisional cascade, including stellar radiative and stellar wind forces. Our models were compared to a suite of observational data for scattered light and thermal emission, ranging from polarisation measurements in the visible to the ALMA radial surface brightness profile at 1.3mm. Most of the data can be reproduced with a planetesimal distribution that has an outer edge at around 40au and possesses a low dynamical excitation. We find a preference for strong stellar winds and for dust grains that consist of a silicate-carbon mixture of moderate porosity. While the SED and the shape of the ALMA profile are well reproduced, the scattered light observations deviate from the models more strongly. This possibly indicates a shortcoming of the scattered light model by spherical grains used. We also discuss the origin of the unresolved central emission detected by ALMA and show that it cannot stem from an additional inner planetesimal belt alone.

#### 12:00 [35] Planet formation in evolving protoplanetary discs

#### Presenter: Dr. BITSCH, Bertram

In this talk, we will present a new model for time evolving accretion discs (Bitsch et al. 2015) and its influence on the formation of planetary cores via pebble accretion and on the formation of gas giants in these discs (Bitsch et al. 2015b, in review). We will also show the influence of the ice to silicate ratio on the structure of the protoplanetary disc and hence on planet formation (Bitsch et al. 2015c, in prep.).

The formation of dust, pebbles, planetesimals and planetary embryos is influenced by the structure of the underlying protoplanetary disc, in particular the profiles of temperature, gas scale height and density. The formation of gas giants is additionally tied to the lifetime of the protoplanetary disc, which is expected to be several Myr. During this time the disc looses mass and changes its structure. This evolution of the disc over several Myr is studied in 2D hydrodynamical simulations featuring viscous and stellar heating as well as radiative cooling. The cooling is influenced by the ice to silicate ratio (through the disc's opacity), which changes the disc structure and hence the formation path of planets. A larger ice fraction results in a larger aspect ratio H/r of the disc at  $r > r_{ice}$  and a smaller aspect ratio for  $r < r_{ice}$ . A smaller ice fraction has the opposite effect (smaller H/r for  $r < r_{ice}$  and larger H/r for  $r < r_{ice}$ ).

During the evolution of the disc planets can form via the accretion of pebbles quite quickly (a few 100kyr) until they reach pebble isolation mass where the accretion of pebbles terminates, allowing for the accretion of gas. During this whole process, planets migrate through the disc either in type-I migration (for planets of a few Earth masses) or in type-II migration, when planets are big enough to open a gap in the disc. We discuss the interplay of pebble and gas accretion in combination with disc evolution and planetary migration on the formation of giant planets as a function of their initial orbital distance where they form, their initial formation time during the disc evolution and the ice to silicate ratio in the protoplanetary disc. We will focus here particularly on the formation of the giant planets in our own solar system.

### 12:15 [75] Connecting the composition of exoplanets and their atmospheres with protostellar disk chemistry

Presenter: Prof. PUDRITZ, Ralph

The chemical composition of exoplanets and their atmospheres is arguably the most important ingredient in determining their mass-radius relation and their atmospherics properties. The initial chemical composition of exoplanets is a consequence of their accretion history as they migrate through their natal protoplanetary disks accreting both solids and gases as they build and move through their host disks. We have recently constructed a theory of planet formation that emphasizes the role of planet traps in regulating the slow inward drift of accreting planets. These dynamical traps are disk inhomogeneities in density and temperature such as ice lines, dead zone boundaries, and heat transition radii where disk heating switches from disk viscosity to radiative heating from the central star. In this contribution we present results on both the solid and gaseous composition of planets such as warm Jupiters and SuperEarths as they move along "evolutionary tracks" in the mass- semimajor axis diagram that has come to characterize exoplanetary populations. We show that the solid composition of planets depends to a large degree on whether or not they formed on particular traps (eg. ice lines). We compute the non-equilibrium chemistry of protoplanetary disk models and show how the initial protoplanetary atmospheres depend on their accretion history in protoplanetary disks. We link our models with observations of planetary atmospheres associated with hot Jupiter and SuperEarths.

## PROTOPLANETARY DISK EVOLUTION AND SOLAR SYSTEM (II): Solar System (comets, meteorites, asteroids and links to Solar System formation) - (14:00-16:15)

#### Solar System (comets, meteorites, asteroids and links to Solar System formation)

time [id] title

#### 14:00 [106] Complex molecules in comets

Presenter: Dr. BOCKELEE-MORVAN, Dominique

A review of the composition of cometary ices will be presented, including recent discoveries of complex molecules. Abundances of complex organics in comets will be compared to values measured in hot-cores and hot-corinos, and to results of chemical models of proto-planetary disks.

#### 14:25 [34] The volatile inventory of comet 67P/Churyumov-Gerasimenko from Rosetta/ROSINA

#### Presenter: LE ROY, Léna

Comets are believed to belong to the most pristine bodies in the solar system. The study of their composition can therefore give us important clues about the processes that occurred during the solar system formation [1].

The composition of cometary atmospheres has been investigated remotely and by in situ spacecraft measurements. Until now more than twenty molecules have been identified [2].

The European Space Agency's Rosetta mission gives us a unique chance to probe and study the composition in the inner coma of comet 67P/Churyumov-Gerasimenko (67P/CG). Rosetta is the first mission to orbit a comet and to land a module on its surface [3]. The Rosetta orbiter follows the comet from ~3.5 AU through perihelion and out again to ~3.5 AU over a time-span of more than 2 years.

On board the Rosetta spacecraft several instrument aim to study the composition of 67P/CG (atmosphere and/or nucleus). Among them, the ROSINA (Rosetta Orbiter Sensor for Ion and Neutral Analysis) experiment [4] is dedicated to study the composition and the dynamics of 67P/CG's coma. ROSINA consists of a suite of three instruments: a pressure sensor (COPS: COmetary Pressure Sensor) and two mass spectrometers: the Reflectron Time of Flight mass spectrometer (RTOF) and the Double Focusing Mass Spectrometer (DFMS). The two sensors are complementary. RTOF has a large mass range and can record mass spectra at high time resolution; whereas DFMS has a high mass resolution (m/dm = 9000 at FWHM at 28 u/e). DFMS is a traditional mass spectrometer that combines an electrostatic analyzer for energy analysis with a magnet for momentum analysis. To date, DFMS is the highest mass resolution mass spectrometer in space. It is able to resolve CO from N2 at m/q= 28 u/e or 12CH and 13C at m/q= 13 u/e [4]. This allows to measure many isotopes in different molecules, such as the deuterium and oxygen isotopes in water [5].

Since August 2014, ROSINA is monitoring the volatiles in 67P/CG's coma [5, 6, 7, 8]. In October 2014, to prepare for the lander delivery, the Rosetta spacecraft flew in terminator orbits at an unprecedented close distance (10 km) from the nucleus during roughly two weeks. The total neutral density was high during these measurements, which enabled the detection of minor species in the coma. In March 2015 the spacecraft performed a close flyby with closest approach at 8 km from the center of the nucleus. During this period, we observed even higher densities but for a very short time and numerous neutral species have been detected for the first time in comets. In our presentation we will present some of these molecules and compare our results with the composition in the interstellar medium.

#### References

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#### 14:50 [3] Revealing the Ancient Heritage of Solar System Ices

Presenter: Dr. CLEEVES, L. Ilsedore

Identifying the formation history of the solar system's water and simple organic content is central to understanding the conditions that fostered life in at least one planetary system, and how common such conditions are elsewhere. A key clue in this pursuit is that both water and organics in primitive solar system bodies are characteristically enhanced in their deuterated isotopologue relative to standard (D/H), where the organics are typically more enriched than water. This isotopologue signature points to formation in very cold (\$T<50-100\$ K) environments, facilitated by the presence of ionizing agents, i.e., cosmic rays, radionuclide decay, and X-rays. These requirements point to two possibilities: formation within the protoplanetary disk or inheritance from the parent molecular cloud. Using a comprehensive treatment of disk ionization, we find ion-driven D/H fractionation pathways in the disk are inefficient, inhibiting both the formation of deuterated water and organics especially in the midplane. We have also isolated potential chemical explanations for the D/H differences between water and organics. We find that while a significant fraction of water ice was likely inherited from the parent molecular cloud, organics have a much more complex and varied history. Our findings imply that - if the solar system's formation was typical - interstellar water and organic ices are available to all nascent planetary systems.

#### 15:05 [113] Outer solar system formation: first lessons learnt from Rosetta/ROSINA

Presenter: Prof. MOUSIS, Olivier

Comet 67P/Churyumov-Gerasimenko (67P) is a Jupiter Family comet targeted by the Rosetta mission for in-situ analysis of cometary material and properties. The ROSINA (Rosetta Orbiter Sensor for Ion and Neutral Analysis) instrument on board of the Rosetta spacecraft has been analyzing the composition of gases emitted from 67P since August, 2014 [1]. Here we review the different molecular and isotopic measurements that have been performed by ROSINA over the last few months. We discuss the implications of these measurements for deriving some clues on the formation conditions of the outer solar system. For example, the comparison between the N2/CO and Ar/CO ratios measured in 67P [2,3] places important constraints on the structural properties of the icy grains from which the comet was agglomerated. Also, the high D/H ratio measured in 67P, about 3 times higher than the standard SMOW value [4], matches chemical models that predict a monotonic radial increase of the deuterium enrichment profile [5,6] and implies that the comet formed at a higher heliocentric distance than JFCs and OCCs with lower D/H ratios, in agreement with recent dynamical models of the outer solar system [7]. If the low N2/CO ratio measured in 67P [2] is typical of that of planetesimals formed in the outer solar system, this implies that the compositions of Jupiter and Saturn cannot be explained solely via the accretion of these solids during their formation.

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#### 15:30 [107] The cosmic heritage: message from the short lived radionuclide 10Be

Presenter: Prof. CECCARELLI, Cecilia

The Solar System is the result of a long and complex process that transformed an initial diffuse cloud of the interstellar medium into planets, asteroids and comets. Like in the Grimm's tale, we can find some crumbs, left along the process, which can help us to understand the path that lead where we are today. Among them, the short lived radionuclides decay products in meteoritic and terrestrial material provide us with specific information on the first phases of the Solar System birth. In this contribution, we will present a study on the challenging message from the short lived radionuclide 10Be, and the Herschel observations towards young protostars that help to understand what happened to our Solar System.

15:45 COFFEE BREAK

#### Conference summary and open questions - (16:15-16:45)

- Presenters: Prof. CASELLI, Paola

#### POSTER PRIZE + PRIZE WINNER TALK - (16:45-17:00)

#### Exoplanet Atmospheres - (17:30-18:00)

- Presenters: Dr. HELLING, Christiane