1 Scientific justification: Unveiling the chemistry of planet formation

Planets form and obtain their compositions in dust and gas-rich disks around young stars. This process is intimately linked to disk chemistry: (1) disk chemical structures shape and (2) are shaped by planet formation, and (3) molecular emission patterns are often the best and sometimes the only probes available of disk physics associated with planet formation. **With this proposal we aim to map out the chemical structures, explore how ongoing planet formation shape the disk environment, and constrain the disk gas properties, all at planet forming scales.**

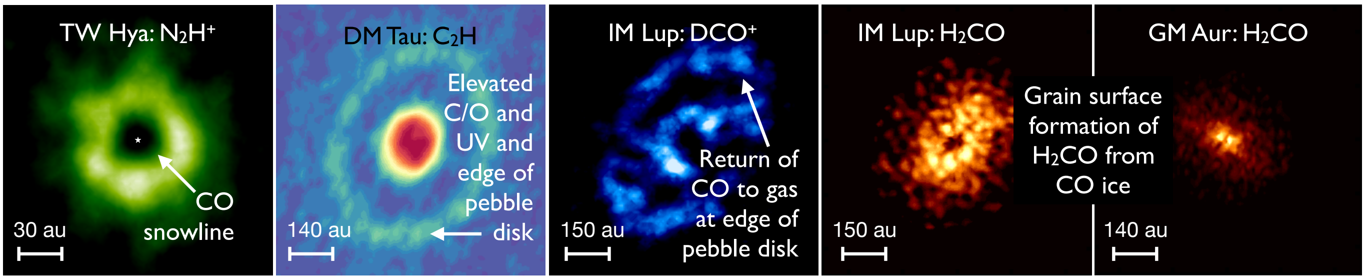

Figure 1: *ALMA observations of chemical sub-structure in protoplanetary disks and their proposed causes. Note that there is clear chemical differentiation both within and between disks (cf. H_2CO and DCO^+ in IM Lup, and H_2CO in IM Lup and GM Aur). (Qi+ 2012, Bergin+ 2016, Öberg+ 2015b)*

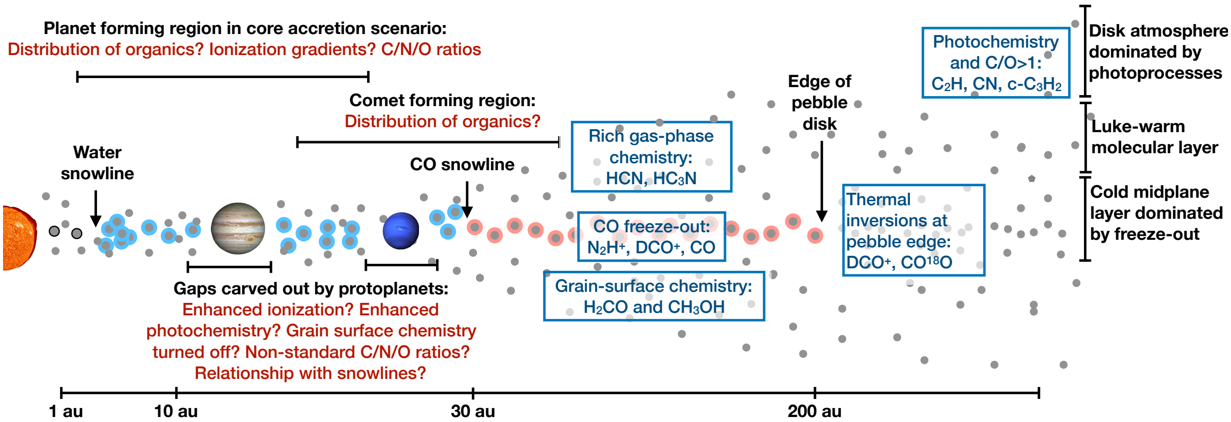

Figure 2: *Illustration of major disk structures (black), observed chemical structures in the outer disks and the molecules that probe them (blue), and the unknown chemical structures in the inner 30 au of disks and unknown chemical responses to disk gaps (red).*

(1) Disk chemical structures shape the efficiency and outcome of planet formation. Planet formation in disks begins with the coagulation of dust grains to form pebbles. Condensation fronts or snowlines in disks of major volatiles (e.g. water and CO) change the efficiency of this process through impacts on grain stickiness and concentration (e.g. Chiang et al. 2010, Gunlach et al. 2011, Pinilla et al. 2016,2017). Chemical gradients across disks, including those induced by snowlines, also regulate the bulk gas-phase and solid-phase compositions of planets and planetesimals (e.g. Lewis 1974, Öberg et al. 2011). Gas-phase C/N/O ratios across the inner disk is of special key interest to the exoplanetary community; the most common interpretive framework of exoplanet compositions attempt to relate present-day atmospheric compositions to disk gas elemental ratio where the planet formed. Finally, the organic inventory of planets and planetesimals is set by the organic composition in disks during planet formation. Over the past cycles ALMA has provided empirical evidence of that planetesimals assembling at different radii will indeed be organic-chemically distinct (e.g. Öberg et al. 2015a, Fig. 1), and that gas-phase C/N/O ratios vary across disks (e.g. Bergin et al. 2016). These constraints all apply to the outer disks, however. To constrain how chemistry shapes the outcome of planet formation we need to address: *What is the gas-phase elemental ratio in the inner*

30 au of the disk? How does the organic chemical composition vary across the comet forming zone? (Fig. 2).

(2) Planet formation shapes the disk chemical environment. The basic chemical structure in disks is set by radial and vertical gradients in temperature, radiation flux, and density. Vertically, this results in a three-layer structure composed of a photochemistry-regulated atmosphere, a molecular intermediate layer, where gas-phase and grain-surface produced molecules thrive, and a cold midplane characterized by molecule freeze-out, resulting in a sequence of snowlines (Fig. 2). The vertical outer disk structure has been probed by multi-line observations, confirming that most molecular emission to luke-warm 20-40 K disk layer (e.g. Öberg et al. 2017, Loomis et al. subm.), and direct observations of vertical emission structure (e.g. Rosenfeld et al. 2013).More surprisingly, ALMA has revealed that radial chemical structures are very sensitive to the pebble disk structure, especially to the edge of the pebble disk as traced by millimeter emission. Here DCO^+ and $C^{18}O$ sometime reappears after having been depleted in the outer pebble disk, and tracers of photochemistry and high C/O ratios become abundant (Fig. 1–2, Bergin et al. 2016, Öberg et al. 2016).

Does the distribution of pebbles shape the chemical structure in the inner disk as well? Recent ALMA observations of disk sub-structure in a large sample of disks (PI: Andrews) reveal that pebble disk sub-structure at the 10 au scale is ubiquitous in protoplanetary disks (Huang et al. in prep, Fig. 3). This most exciting possible origin of the observed gaps, rings and spirals are ongoing planet formation. Based on outer disk chemical changes at the pebble disk edge, and chemical model predictions, dust sub-structures will locally change the chemical environment. In which ways, and how sensitive this is to the details of the substructure is unknown, but *molecular abundances regulated by availability of grain-surfaces (e.g. H_2CO), UV photons, temperature and ionization are likely to be different in the gaps compared to the surrounding regions.*

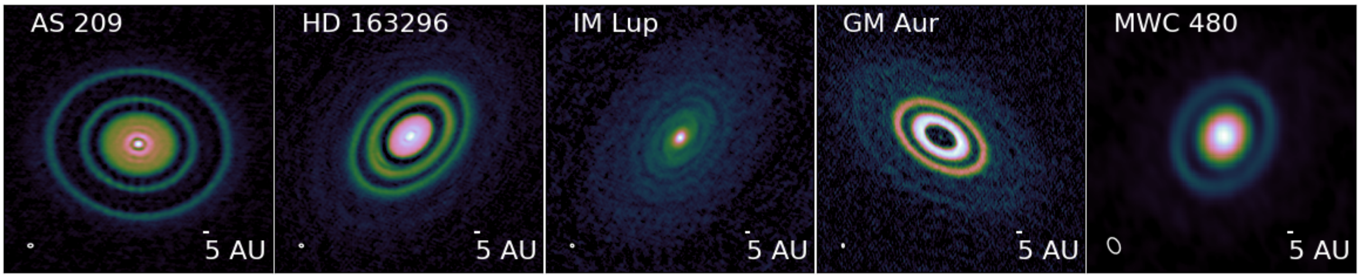

Figure 3: *Gallery of ALMA images showing disk sub-structures at ∼0.05–0.1" angular resolution: nested rings around AS 209, inner disk + two large rings around HD 163296, the spiral in IM Lup, small disk + two large two rings around GM Aur, and inner disk+compact ring around MWC 480.*

(3) Molecular emission probe planet formation physics. In addition to shaping the outcome of planet formation, disk chemical structures encode information about disk ionization, density and temperature structures, and dust and gas dynamics, all of which are key to anchor models of planet formation. In particular, isotopic fractionation patterns (e.g. D/H ratios) can be used to probe the history of key volatiles; in the Solar System isotopologue ratios in Earth's water and in comets are frequently used to make claims about their origins, but these claims are tenuous without better constraints on the distributions of isotopologues in disks. Molecular emission lines also constitute our only probes of gas masses, radial and vertical temperature structures, constraining what kind of planetary system could form in disks, and disk kinematics related to ongoing planet formation. Different molecular probes have been put to the test in outer disk regions (e.g. Cleeves et al. 2015). Exploring the inner disk regions with chemical probes is new territory and we therefore do not know: *What is the gas content of the gaps seen in Fig. 3 and what is that telling us about the gap origins? How does gap opening and spirals affect the ionization and temperature structures of disks?*

We propose to address all the above questions through a Large Program aimed at elucidating the chemical structures in disks at the scales of planet formation. Only

ALMA has the requisite sensitivity and spatial resolution for such a study. **Why now?** A few months ago the ALMA Large Program on high-spatial resolution dust observations toward a large sample of gas-rich disks was completed, revealing that dust sub-structure in disk is ubiquitous; the impact of dust sub-structure on chemistry is then urgent to explore. Contemporaneously, our ALMA disk chemistry studies have demonstrated which molecules are observable in disks, and the necessity of constraints on excitation and dust opacity to interpret molecular emission patterns. The path is thus clear for a well-informed LP. **Why a Large Program?** A large program is required to comprehensively map out the chemical structures in a small sample of disks in multiple ALMA bands; in <100h we can survey ∼5 disks in depth. We think a small and deep survey is the right path for a disk chemistry LP; it avoids the risk of basing conclusions on a single disk, which may not be representative, and larger surveys are by necessity more shallow and will lack the sensitivity to explore the most interesting disk regions for planet formation, especially the inner disk midplanes.

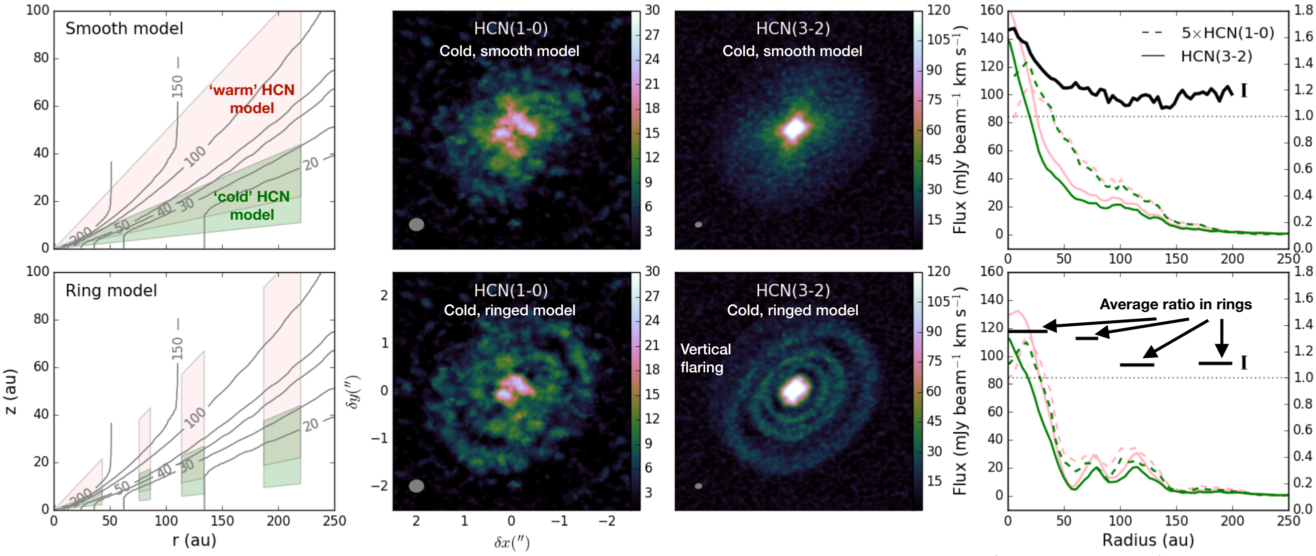

Figure 4: *Simulation of HCN line emission toward one of our disks (HD 163296) using the requested resolutions and integration times in B3 and B6 and total line fluxes from existing observations (Graninger et al. 2014, Bergner et al. in prep.). Upper panels: HCN is smoothly distributed at either high (red) or intermediate disk heights (green). Lower panels: HCN follows the dust sub-structure (Fig. 2), demonstrating that we can address questions on chemistry-dust relationships. The right hand panels show the radial profiles for the different models and that the relative fluxes 1–0 (B3) and 3–2 (B6) lines can be used to constrain the molecular emission layer (black lines). Note that the vertical disk structure can be directly resolved in B6.*

2 Description of observations: Disk chemistry at 0.1” scales

Immediate objectives: We propose to map the chemistry in 5 disks at 0.1” in B6 lines and 0.2” in B3 lines, corresponding to radial scales of 7-15 au at distances of 122–161 au (Table 1). The result will be a data set that reveals the chemical environment within which planets form at unprecedented detail (Fig. 4) , including the radial and vertical distributions of organic molecules and key chemical probes, and the relationship between chemistry and dust sub-structure:

What is the interplay between dust and chemical structures? Disks display substantial sub-structure in dust emission at scales of a few to 10s of au (e.g. Andrews et al. 2016, Isella et al. 2016, Perez et al. 2016, Fig. 3); which molecules correlate, which ones anti-correlate, and which ones display mixed or no dependence on dust sub-structure? By combining B3 and B6 lines we will map out these relationships, and constrain the physics and chemistry that drive them. By covering both T Tauri and Herbig Ae stars we will also provide first constraints on how the central star interacts with dust sub-structure to shape the inner disk chemistry.

What are the vertical distributions of molecules in disks? Protoplanetary disks are flared (see e.g. Avenhaus et al. 2018). We will probe the vertical chemical disk structures by directly resolving them (Rosenfeld et al. 2013), and through line excitation analysis (Fig. 4).

How are organic molecules and the volatile elements distributed in the planet forming zone? We will map the distributions of organic molecules of especial interest to origins-of-life chemists, i.e. cyanides, small carbon chains, and molecules involved in ice chemistry (e.g. Powner et al. 2009), tracers of isotopic fractionation chemistry, and probes of gas-phase C/N/O elemental ratios in the planet and comet forming disk regions.

Disk sample: We propose to target five disks (Table 1). The sample size enable us to cover all families of disk sub-structure identified by ALMA, and both T Tauri and Herbig Ae stars. The disk were primarily chosen based on their sub-structure discovered by ALMA: spirals (IM Lup), thin and thick nested rings at multiple scales (AS 209, HD 163296 and likely MWC 480), and a small (au scale) disk with one or several outer disk rings (GM Aur). The disks were further selected to minimize cloud obscuration (AS 209 and IM Lup are somewhat cloud-contaminated in ^{12}CO, but not in the targeted molecular lines), and to have inclinations of 40-50° to optimally resolve radial and vertical structures (Rosenfeld et al. 2013).

Table 1: Disk sample data

Source	Star	RA	Dec	d [pc]	i [°]	Dust sub-structure
IM Lup	M0	15 56 09.18	-37 56 06.1	161	50	Spirals + rings
AS 209	K5	16 49 15.30	-14 22 08.6	126	38	Narrow (<10 au) nested rings
GM Aur	K5	04 55 10.98	+30 21 59.5	140	49	Large gap + rings
MWC 480	A4	04 58 46.27	+29 50 37.0	142	37	Nested rings?
HD 163296	A1	17 56 21.29	-21 57 21.8	122	49	Thick (10–20 au) nested rings

Table 2: *Molecular line targets – secondary targets (not used for time requests) in italics.*

Set-up	Line targets
B3-1	1-0: HCO^+, $H^{13}CO^+$, HCN, CCH, *$H^{13}CN$, $HC^{15}N$. HC_3N 11-10*
B3-2	1-0: ^{13}CO, $C^{18}O$, *$C^{17}O$*, CN. *CS 2-1*
B6-1	2-1: ^{12}CO, ^{13}CO, $C^{18}O$. 3-2: DCN, H_2CO, *N_2D^+. CH_3CN 12-11*
B6-2	3-2: HCN, CCH. *HC_3N 29-28, c-C_3H_2 6-5, 7-6*

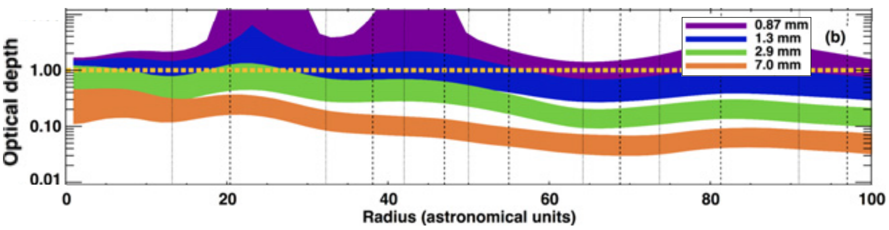

Figure 5: *Opacities in B6 (blue) and B3 (green) for the HL Tau disk, demonstrating the need of B3 observations to see the disk midplane inside of dust rings (from Carrasco-Gonzalez+ 2016)*

Spectral line targets: We propose to observe the five disks in: 1) Molecular gas tracers ^{12}CO 2–1, ^{13}CO 1–0/2–1, $C^{18}O$ 1–0/2–1, and $C^{17}O$ 1–0. Despite its shortcomings, CO remains the best probe of the gas radial and vertical gas structure (Molyarova et al. 2017). 2) Molecular ions. HCO^+ is the predicted main molecular ion and by targeting it and its optically thin isotopologue in B3 we will be able to probe ionization both between and inside dust rings. 3) Small organics. C_2H, HCN and H_2CO are our primary targets, but we also observe $H^{13}CN$, HC_3N, CH_3CN. 4) Deuterated and ^{15}N isotopologues of HCN, which are used to assess isotopic fractionation. 5) C/O/N tracers C_2H, HCN and CO isotopologues, which together constrain the gas-phase C/N/O ratio (Du et al. 2015); all are covered both in B3 and B6, which will give us access to these ratios both in the disk midplane and the smallest scales. 6) Photochemistry tracers CN and C_2H. These lines are covered by 4 spectral set-ups (Table 2), which were selected to address the largest number of science goals in the smallest number of settings. *We stress the importance of covering lines in both B3 and B6; the former offer* *the only path to observe the midplane inside of dust sub-structure (Fig. 5), while the stronger B6 lines enable use to probe smaller radial and vertical scales, and both are needed to constrain molecular excitation.*

3 Data analysis: from molecular lines to chemical structures

Our analysis strategy is to obtain initial qualitative constraints directly from the data, followed by quantitative extraction of chemical structures, and interpretation in light of model predictions.

Data driven analysis: Our first goal is understand the diversity of chemical structures across disks at 10 au scales that include dust sub-structure. We will image all lines and compare the spatial morphologies of strongly detected molecular lines and dust along the plane of the disk. We will pay special attention to the relative morphologies of B3 and B6 lines, which informs us on where dust opacity affect line emission structures. We will also explore vertical distributions of line emission using 1) line emission spatial patterns across velocity channels (Rosenfeld et al. 2013), which for moderately inclined disks provides strong constraints on the disk height of the emitting layer, and 2) B3 and B6 line ratios, taking into account dust and line opacity as needed.

Molecular retrieval models: We will retrieve chemical abundance structures from line emission profiles through forward-modeling, using molecular parametric abundance profiles informed by the qualitative analysis above and astrochemistry models, and using constraints on disk density and temperature structures from dust and CO observations (e.g. Guzman et al. 2017).

Astrochemical models: The obtained radial and vertical abundance structures and their dependence on dust sub-structure and stellar parameters will be interpreted using astrochemistry models. Within the team we have access to three state-of-the-art astrochemistry disk codes (developed by Cleeves and Bergin; Walsh; and Furuya, Aikawa and Hideko) optimized to model different aspects of the disk chemistry including structure-chemistry relationships, photochemistry, isotopic fractionation, gas dynamics, and complex organic formation (Fig. 6). In addition to comparing generic models to observed chemical structures, we plan to develop disk-specific models to quantitatively test the predictive value of existing astrochemistry codes, and to develop them further where they are currently lacking to better predict chemical evolution during the entire epoch of planet formation.

4 Scheduling feasibility

The proposed program requires 5h per spectral set-up and disk in B3 and B6, resulting in a total time request of $\sim$100 h. The B3 observations are mostly (80%) in C43-7 with short baselines obtained in C43-3. The B6 observations are mostly in C43-6 with short baselines in C43-3. The total time in C43-3 is <20h distributed between two LST ranges, well below the available 10 h per h in LST. in C43-7 there is $\sim$10 h available per h LST in the relevant LST ranges and our total requirement of 40 h is readily scheduled with the available time for LP. Finally, we need $\sim$40 h in C43-6. Availability in the relevant LST ranges are $\sim$13 h per LST h and we are thus within the allowed limit for LPs.

5 Data products

We commit deliver the following data products to the community:

1. Matched filter response spectra of all data cubes in all disks, where the filter is data-driven, based on strong lines in each disk, which will immediately tell the community which molecular tracers are observable at these spatial scales.
2. Self-calibrated and imaged data cubes of all targeted lines towards all the disks together with standardized scripts that enables the community to reproduce the spectral-image cubes from the calibrated data delivered by ALMA.
3. Extracted spectra, moment 0 maps using Keplerian masks, and radial profiles of all targeted lines and disks, together with the scripts used to produce these high-level data products.

6 Management plan

The team is lead by 5 co-PI's who each will be responsible for one science area and for the complete calibration, imaging, and initial analysis of one of the five disks. To ensure that the disks are speedily and uniformly self-calibrated and imaged we will adopt the following plan: Each of the co-PI's has committed to themselves or an experienced student or post doc lead the self-calibration and imaging on one of the disks. Several different calibration and imaging strategies will be explored, but we will ensure that the final data products are uniform and easy to interpret. To ensure a smooth process, we will have bi-weekly telecons within the core-calibration team to share lessons learnt and reach consensus on the strategy that we adopt as a team. Öberg will be responsible for organizing the telecons. Once the final strategy is agreed upon, each of the teams will proceed and upload calibrated image cubes as they become available on a dedicated github. We imagine the calibration/imaging step will take at least a few months.

Low-hanging fruit discovered during the data imaging steps of individual disks will be published by the co-PI's team as expediently as possible unless otherwise agreed upon. Öberg and Huang will cover GM Aur, which Huang already has experience on from a separate project focused on disk structure, Bergin and Cleeves will be responsible for IM Lup that has been extensively researched by Cleeves on larger scales. Guzman will lead the work on AS 209, whose dust structure she is intimately familiar with, Walsh and post doc will lead the work on HD 163296, and Aikawa and post doc on MWC 480.

Öberg will be responsible for publishing an overview of the project results to the community. Beyond this, each of the co-PI's will lead the exploration of one of the five science questions, which each require data from the full disk sample. Guzman will lead the exploration of small organics in disks, building on her experience with constraining HCN and H_2CO distributions on larger scales in disks. Walsh will lead the extraction of distributions of the most complex molecules in this study: HC_3N, CH_3CN and c-C_3H_2, and the modeling of their chemistry. Aikawa and Furuya will lead the extraction and modeling of deuterated molecules. Bergin will lead the extraction and modeling of C_2H, CN and CO and the interpretation with respect to C/O ratios, PDR chemistry and their connections to dust structures. Öberg and Cleeves will lead the exploration of ion chemistry and its relationship to dust structure. Each science team is expected to connect via skype on a bi-weekly basis once the initial calibration work is complete. In addition the entire team will connect via skype on a bi-monthly basis and in yearly face-to-face meetings.

7 References

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