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RESEARCH PROPOSAL

Heat and the fate of interstellar molecules in planet-forming regions

Planets are born from a grand chemical odyssey—a story that begins in a cloud of gas and dust, brimming with chemistry, which collapses to form a protostar. The material surrounding this young star develops into a protoplanetary disk, which eventually coalesces into planets and planetesimals. Many interstellar molecules either form or condense on dust grains, creating a frozen coating harboring a complex chemical inventory. As the environment evolves from clouds to disks, these ices undergo transformations that shape what molecules are available for incorporation into planetary bodies. This raises two fundamental questions: *which ingredients survive this interstellar journey?* and *in what chemical and physical states are they available for forming planets and planetesimals?* The answers lie in understanding the physicochemical processes that govern ice evolution, achievable only though a multidisciplinary approach bridging astronomy and chemistry. I am an expert on this intersection. My research combines astronomical observations, which constrain the molecular history of interstellar space, with laboratory experiments that elucidate the mechanisms behind these observed outcomes. In my PhD, I applied this approach to trace the origins of the molecular building blocks that drive protoplanetary chemical complexity [1, 2, 3, 4, 5]. As a 51 Pegasi b fellow, I will focus on uncovering their *fate* before incorporation into planets and planetesimals. Specifically, I will establish how thermal heating by the protostar influences planetary composition. A key aspect of this process is the sublimation of volatiles, which dictates their partitioning between solids and gases. I will explore three interconnected projects at the forefront of this challenge: how the partitioning is affected by entrapment, how it is affected by chemistry, and how sublimated volatiles can accurately probe the ice makeup.

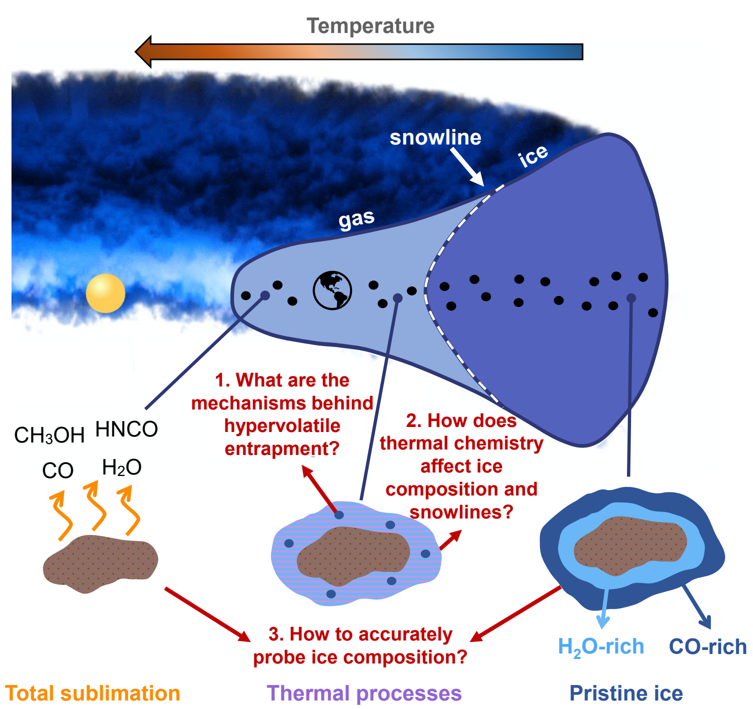

Figure 1: Cartoon of a protoplanetary disk with the key open questions to be answered during my fellowship in red. The insets show the ice structure as a function of temperature, dictated by the distance to the protostar. The pristine ice composition consists of a water-rich layer formed during the early, low density cloud stage, underneath a CO-dominated counterpart produced later, in the cloud cores [7]. Within these layers, different ice species coexist in complex mixtures. Adapted from the original art by T. Birnstiel.

1. Unveiling volatile entrapment mechanisms and their effects on snowlines. The emergence of a protostar generates a temperature gradient that causes distinct sublimation fronts, or snowlines, where specific molecules transition from solid to gas (Fig. 1). Snowlines play a major role in planetary science: they influence grain growth and intimately shape planetary composition [6]. Beyond them, molecules remain frozen and may be incorporated into planetesimal cores, which in turn may deliver these species to terrestrial planets during events such as our Solar System's late heavy bombardments. Within them, molecules exist as gases and may contribute to a planet's atmosphere. Locating snowlines is thus vital for determining the bulk composition and chemical evolution of planetary bodies.

Snowlines are governed by the structure of the parent ice. Molecules that form alongside water—the main ice component [8]—become embedded within it. As temperatures rise, these embedded species more volatile than water can become entrapped in the aqueous ice matrix, unable to escape into the gas phase until the water ice itself desorbs (Fig. 1). Their sublimation behavior in disks is therefore largely dependent on how efficiently they are entrapped. Over the last two decades, laboratory measurements of entrapment efficiencies have provided valuable data for specific matrix-volatile combinations. However, the underlying mechanisms behind this phenomenon remain poorly understood. In particular, heat-induced diffusion may significantly impact entrapment efficiencies, casting doubt on the reliability of laboratory-derived values, where typical heating rates—and thus diffusion kinetics—are orders of magnitude away from representative interstellar scenarios [9]. As a 51 Pegasi b Fellow, I will be the first to utilize cryogenic vacuum apparatuses to systematically constrain the effects of heating rates and ice diffusion on entrapment efficiencies, bridging the gap between lab measurements and *realistic* values that can be incorporated into disk models.

2. Disentangling ice thermal reactions and sublimation during planet formation. The impact of the temperature gradient on the chemical distribution in planet-forming regions is not limited to entrapment; it also induces radial variations in composition by triggering chemistry. Heat promotes diffusion, which favors encounters among reactants, and helps overcome activation barriers, accelerating chemical reactions. This can drastically modify the ice composition, which in turn affects snowlines and consequently the distributions of C, N, O and S between gas and solids [6]. I will work towards disentangling the interplay between chemistry and sublimation during my Fellowship. Experimentally, I will characterize the kinetics of thermal reactions in a sample of model systems and their effects on sublimation, which will guide the interpretation of observed spatial and temperature distributions of key molecules in disks. Salts will be the primary targets of this study: their formation is largely driven by heat, and as typically semirefractory species, they can significantly shift the snowlines of their volatile constituents. Indeed, salts are likely major reservoirs of nitrogen and sulfur in comets [10, 11], playing a key role in protoplanetary chemistry and the prospect of abiogenesis. For the observational component of this project, I will use spatially-resolved data from the Atacama Large Millimeter/submillimeter Array (ALMA) to identify relative snowline positions by comparing emissions from molecules with varying volatilities. I will apply for telescope time as PI and also make use of available archival data. Class 0/I objects will be the testbeds for more evolved planet-forming regions, since their higher luminosities render sublimation fronts observable at scales of tens of a.u., unlike in Class II disks where most snowlines are too compact to be resolved. Ice material appears to be largely inherited throughout disk evolution [12, 13], and thus insights on ice processes from these younger sources should also be applicable to later stages. Moreover, young Class 0/I disks already contribute to planet and planetesimal formation [14, 15], providing a unique opportunity to study the chemical conditions under which these processes begin. In fact, these earlier stages might be the most important period for locking up volatiles in salts [16].

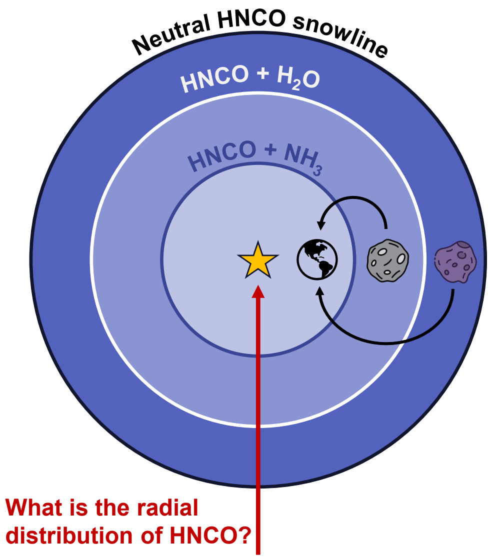

Figure 2: Schematic of the potential HNCO snowlines in a planet-forming disk. Thermal reactions impact the reservoir of HNCO in ices and thus its sublimation, shaping its availability for incorporation into planetesimals that may deliver life's feedstock to habitable-zone planets. Core Project #2 will disentangle the thermal chemistry of HNCO and its resulting chemical structure in disks.

The first system I will study is isocyanic acid (HNCO), the simplest stable molecule containing the four main biogenic elements, and a promising precursor of peptides [17], vital for the emergence of life. HNCO undergoes heat-dependent acid-base reactions with abundant ice components (e.g., H_2O, NH_3; [8]), forming semirefractory salts that can *dramatically* shift its sublimation fronts while retaining a peptide-like moiety. This could significantly impact the development of chemical complexity in icy planetesimals, which in turn may act as the main deliverers of life's building blocks to habitable-zone planets (Fig. 2). I will provide the first *comprehensive* characterization of the HNCO reservoirs and their radial extent during planet formation. Experiments will determine its binding energies and corresponding sublimation fronts across different chemical states, which will be integrated with observations of its spatial and temperature distributions relative to benchmark species.

3. A new framework to observe ice composition. The mixing environment is crucial in shaping the fate of an ice molecule: it defines its nearest partners for reactions and determines its intermolecular interactions, consequently affecting its diffusion and desorption kinetics. Accurately characterizing the ice composition is thus essential to predict the chemical structure and evolution of planet-forming regions. Solid-state observations offer great constraints on major ice constituents; however, their inherent limitations complicate the characterization of mixing conditions and hinder the detection of less abundant ice components. In contrast, gas observations are much more sensitive and less prone to line confusion, offering more detailed insights into the complex nature of ices. Molecular abundances of the gas in inner protostellar envelopes—where ice mantles fully sublimate—provide a direct view of more elusive ice species (like complex organics) and serve as a diagnostic for mixing environments: ice molecules formed over similar timescales experience similar physical conditions prior to sublimation, resulting in narrower abundance distributions among various sources compared to species formed at different timescales (Fig. 3). Methanol (CH_3OH) is often used as an ice probe in the gas, as it is efficiently produced in the CO-rich layer. However, as I argue in [4], it is a poor tracer of early-forming molecules, for which H_2O would be a more appropriate benchmark. As the main ice constituent, water also serves as the ideal reference for comparing the abundances of sublimated species and ice observations. By including different evolutionary stages—from pre- and protostellar sources to comets—these comparisons reveal how ice species may be inherited throughout star and planet formation and ultimately incorporated into planetesimals. Recent James Webb Space Telescope observations provide direct evidence that gaseous water column densities in inner protostellar regions likely reflect the actual ice content [18], highlighting the promising potential of using it as an ice probe in the gas phase. Yet, such comparisons have never been explored.

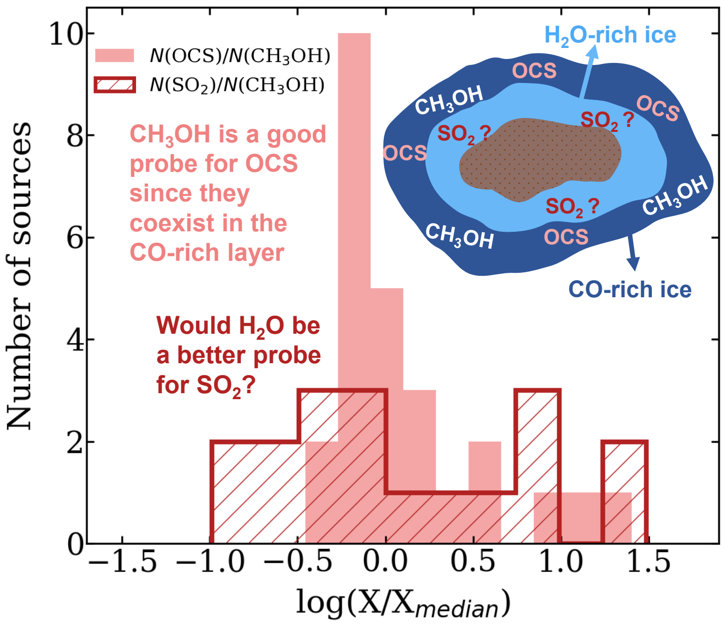

Figure 3: Gas abundance distributions of OCS and SO_2 with respect to CH_3OH in inner regions around massive protostars (adapted from Santos et al. 2024b, [4]). The narrow distribution of OCS/CH_3OH suggests that both species coexisted in a similar ice environment prior to sublimation. In contrast, the ice environment of SO_2 is still debated, and cannot be constrained by the large distribution of SO_2/CH_3OH. Comparisons with H_2O in Core Project #3 will pinpoint the main ice phase of SO_2.

As a 51 Pegasi b Fellow, I will trace the chemical history of target species by using water as a probe for their abundances post sublimation, which will enable more accurate comparisons to ice observations. I will also determine the ice environment of key species for which this is still unclear by comparing abundance distributions with both standards, CH_3OH and H_2O. Minor isotopologues (e.g., $H_2^{18}O$) will be used to avoid issues such as telluric contamination. The first deliverable will be a proof of concept, using publicly available ALMA data to put initial constraints on ice environments and inheritance. However, since most existing observations have not targeted both benchmarks simultaneously, I will seek additional data from ALMA and other interferometers to observe a broad range of molecules alongside both water and methanol, striving for a more refined analysis with a larger sample size and free of biases from different observation conditions. Ultimately, this project will establish a new framework for accurately constraining ice composition and inheritance by planetesimals, providing a solid foundation for predicting the chemical structure of planet-forming disks.

Timeline and risk mitigation. Table 4 outlines the key milestones of the core projects. Experiments will adhere to safety policies with appropriate protective equipment and emergency protocols. Observing proposals will be submitted prior to the fellowship and every year thereafter. In the event of unsuccessful proposals, archival data can be utilized.

Conclusion. Overall, I aim to elucidate the ingredients available for forming planets in our Solar System and beyond by deciphering the fate of ice molecules upon thermal processing. My unique set of skills that combines laboratory experiments and astronomical observational, as well as my interdisciplinary background, sets me apart and equips me to succeed in this endeavor. This is a golden era for this research: cutting-edge vacuum and cryogenic techniques allow us to simulate interstellar environments with high fidelity, while state-of-the-art telescopes offer unprecedented resolution and sensitivity for observations. In the long term, I anticipate my work as a 51 Pegasi b Fellow will significantly enhance our understanding and offer new tools for exploring the chemical structure of planet forming regions and the pathways to habitable worlds—a key challenge highlighted in the 2020 Decadal Survey [19].

Core Project	Milestone	Year 1		Year 2		Year 3	
1. Unveiling volatile entrapment mechanisms and their effect on snowlines	**Calibration experiments:** flow and deposition rates, effective volatile:H_2O mixing ratios						
	Core experiments: TPDs with various heating rates, isothermal experiments						
	Data analysis: determining entrapment efficiencies as a function of heating rate, isothermal diffusion timescales						
	Writing paper(s)						
2. Disentangling ice thermal reactions and sublimation during planet formation	**Calibration experiments:** flow and deposition rates, effective HNCO:base (H_2O, NH_3) mixing ratios						
	Core experiments: TPDs of pure HNCO and mixtures (HNCO:H_2O, HNCO:NH_3, HNCO:H_2O:NH_3)						
	New or archival ALMA data reduction						
	Data analysis: experimental diffusion rate constants and binding energies, observational spatial / temperature distributions						
	Writing paper(s)						
3. A new framework to observe ice composition	New or archival ALMA / NOEMA / other data reduction						
	Data analysis: abundance distributions of key species (e.g., SO_2) relative to H_2O and CH_3OH, comparison with pre- and protostellar ices and comets						
	Writing paper(s)						

Figure 4: Proposed timeline with experimental and observational components shown in blue and pink, respectively. TPD stands for temperature-programmed desorption experiments, i.e., studying ice sublimation by warming up the substrate at a constant rate. Planned timeframes for data reduction and analysis of observations can be adjusted in case proposals are accepted during Year 1 or 2.

References:

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