English Summary

Humanity has always wondered about its origin and place in the Universe. Our ancestors turned to the skies and searched for answers in the stars. Countless myths and legends have permeated across the great civilizations of the past and served as an explanation to fundamental questions about the origin of the Universe and humankind. It has been only recently that modern astrophysics tried to employ rational thinking to explain the origin of Earth and life within the Solar System.

The most widely accepted star (and planet) formation theory starts with a gravitationally unstable molecular cloud of gas and dust. As the cloud collapses under its own gravity, a disk quickly forms as more distant material falls in with larger amounts of rotation (or angular momentum, as physicists call this) . This disk is initially embedded in an envelope of gas and dust. After ~ 0.5 Myr the envelope is cleared out by outflows, driven by the central star, that pierce a cavity within the envelope and leave behind a disk. It is in this circumstellar disk where planets are thought to be formed, thus bearing the name of protoplanetary disks. These disks have been detected around many young starts at different evolutionary stages with very different physical and chemical properties.

The gas and dust content of protoplanetary disks can be probed by observing spectral lines from molecules in the gas-phase and the thermal radiation emitted by the dust resulting in a continuum spectrum. During their typical life span of ~ 10 Myrs the disk undergoes many dynamical processes that transform its structure, eventually leading to the formation of planets and the dissipation of the gas. In addition, protoplanetary disks exhibit rich chemistry mainly driven by ultraviolet and X-ray radiation that may be intrinsically connected to the physical evolution of the disk components (see Fig.8.1). The aim of this thesis is to provide an explanation for the observed morphology of the emission of major nitrogen-, oxygen- and carbon-bearing molecular species by comparing them to the morphology of the dust density profile. In particular, this thesis sets to answer two questions:

- Where are the main oxygen- and nitrogen-bearing species, namely water and ammonia, located within planet-forming disks?
- How do physical structures, such as temperature gradients and substructures in the density of the dust caused by grain evolution processes, relate to the formation and chemistry of common molecular species?

This Thesis

Chapter 1 of this thesis gives an overall introduction of star formation theory and protoplanetary disks with an emphasis on the dust evolution process and the different chemical regimes within disks. The analysis is focused on two well-studied protoplanetary disks, TW Hya and HD163296. Both disks are excellent laboratories because of their proximity and their massive and bright disks. This thesis uses both infrared data from the *Herschel Space Telescope* and (sub)millimeter data from the Atacama Large Millimeter Array (ALMA). *Herschel* was equipped with a 3.5 m single mirror and had three instruments that covered wavelengths ranging from ~50 μm to ~600 μm. Data from the key program "Water In Star-forming regions with Herschel" (WISH), taken with the HIFI instrument on board *Herschel* were used in this work. ALMA is a radio telescope consisting of sixty six antennas with unprecedented spatial resolution and sensitivity that was used to observe both the continuum and line molecular emission presented in this thesis toward our sources.

In Chapter 2, ALMA observations at a wavelength of 1.3 mm are used to investigate where grains of about 1 mm in size are located in the disk around TW Hya. In planet forming disks, small grains (~ μm) stick together and grow into larger grains (mm, cm, and beyond) to ultimately form planets. While μm-sized grains are well coupled to the gas, larger grains will drift inward due to the friction with the gas. The observations show that the mm-sized grains are found out to ~47 AU from the star, after which their amount rapidly drops. Such a steep drop is predicted by theoretical calculations of grain growth and their transport in the disk. However, for typical realistic dust evolution models of T Tauri disks, the observed extent of the grains and their total amount are too large for a disk of 8-10 Myrs. Possible explanations for this include a much higher initial disk size and mass, a dust density gap stopping the radial migration of the mm-sized dust opened by an unseen planet companion or a local overproduction of mm-sized grains aided by the presence of icy grains in regions where CO is frozen out that grow more efficiently than

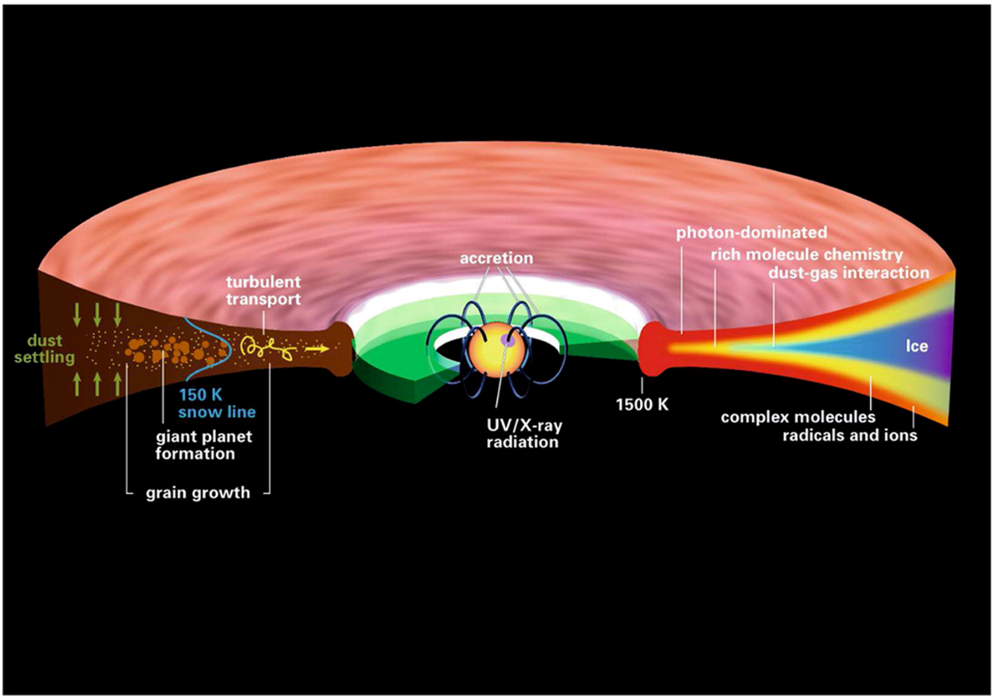

Figure 8.1: Cartoon of dust evolution and chemical regions in the disk. Figure from Henning & Semenov (2013).

bare dust grains.

Chapter 3 presents the very first detection of ammonia toward a planet forming disk. The o-NH_3 1_0–0_0 line was observed with the HIFI instrument on board *Herschel* together with emission lines of o-H_2O and p-H_2O in TW Hya. Four different models for the distribution of these molecules are explored assuming that water and ammonia ices are intermixed and released to the gas-phase simultaneously. Only the most compact and settled distribution of both water and ammonia in the gas-phase, following the millimeter continuum emission radial extent of $r \lesssim 60$ AU, is consistent with the ammonia to water ratio found in the gas between the stars of our galaxy and Solar System bodies of ~ 5%-10%. Other configurations, at larger radii or heights, can only be reconciled with the interstellar and Solar System values if additional formation pathways of ammonia are invoked. The derived gas-phase reservoir of ammonia and water in any of this models is only a tiny fraction of the estimated total reservoir, indicating that most of these molecules are locked up in ices.

The cold gas environment of planet forming disks is expected to host a large amount of deuterium-bearing species such as NH_2D. Chapter 4 analyzes both *Herschel* data of the o-NH_3 1_0–0_0 line and ALMA data of the p-NH_2D 1_0–0_0 line toward the disk around HD 163296. Both resulted in non-detections given their modest integration times. This chapter explores two different radial distributions of gas-phase o-NH_3 and p-NH_2D to put limits on their line strengths and total masses. The upper limits derived for the total mass of gas-phase o-NH_3 and p-NH_2D towards this disk are ten times lower than the values toward the similar-mass disk of TW Hya, derived in Chapter 3 for the preferred model, assuming a NH_3/NH_2D ratio of 10% . This suggests that the disk around HD 163296 is NH_3-poor by at least a factor of 5 compared to the disk around TW Hya. Other nitrogen-bearing species detected towards these disks show different relative amounts than those found for ammonia. This suggest that the difference observed in the total mass of the gas-phase o-NH_3 between these disks is due to its formation pathway and not an overall lack of elemental nitrogen.

The focus of Chapter 5 is the analysis and radial characterization of three simple deuterated species toward a planet-forming disk. DCO^+, DCN, and N_2D^+ were observed and detected in Band 6 with ALMA toward the disk around HD 163296. This chapter translates the radial emission profile of these three molecules to radial densities under simplifying assumptions. The DCO^+ radial emission can be reproduced by a model with three consecutive radial regions and different constant abundances from ~50 AU to ~ 316 AU with two radial breaks at ~118 AU and ~ 245 AU. The first two radial regions of the best-fit model of the DCO^+ emission correlate spatially with the best-fit models describing the radial emission profiles of DCN and N_2D^+. This can be interpreted as a reflection of the fact that there are multiple ways to inject deuterium into the chemistry. One path operates only at the lowest temperatures, and produces N_2D^+; another operates at slightly higher temperatures, and produces DCN. DCO^+ forms through both paths. The origin of the third region of DCO^+ emission at ~260 AU is unknown but it could be tracing higher temperatures allowing CO to evaporate at large radii, where it can react to form DCO^+.

Chapter 6 tries to reproduce the observed DCO^+ emission presented in Chapter 5 using a more sophisticated, but still simple network of chemical reactions for the formation of DCO^+ in cold environments and a parametric model for its formation in warm environments. The DCO^+ emission is reproduced by a model with a CO abundance of $2{\times}10^{-7}$, in regions where the gas temperature exceeds 19 K, and a contribution from the warm environment formation of 20% in regions where both formation pathways are active. At larger radii, the extent and shape of the DCO^+ emission can be reproduced by considering a temperature gradient similar to those predicted by models of dust grain evolution in the presence of inward radial migration of mm-sized dust grains.

Overall Conclusions

The analysis presented in Chapters 3 & 4 provides an answer to the first question this thesis sought to answer. The gas-phase water and ammonia in TW Hya follows the location of their icy reservoir trapped in larger bodies that have settled and drifted inwards. The location of this reservoir is set by the radial drift of grains that have undergone some growth, and subsequently were incorporated in larger rocks. This scenario can be confirmed by observing NH_2D and HDO toward TW Hya and HD 163296. Chapters 5 & 6 draw conclusions on the effect of physical structures on the distribution of simple molecules. Temperature-sensitive species, such as DCO^+, can trace substructures in the temperature profile of planet-forming disks. While the most important factor in the disk's temperature structure is the illumination by the central star, substructures resulting from grain growth, settling and drift modify the temperatures. Species like DCO^+ can be used to indirectly trace the impact of grain evolution on the disk's morphology. The inverse process, i.e. the impact of the the location of simple molecules on dust evolution, is explored in Chapter 2 and can be studied by comparing the shape of the millimeter continuum emission and the location of the snowline of main molecular species such as CO. New infrared and visible light instruments in facilities such as the future James Webb Space Telescope (JWST) or the Extremely Large Telescope (ELT) will be able to observe key molecules in the warm environments of the disk, ice features and resolved scattered light emission allowing us to distinguish the different scenarios explored in this thesis. Large surveys of planet forming disks would help to average out the differences between individual sources and bring forward the general trends in their structure and evolution leading to a comprehensive understanding of the planet and star formation processes.