Hot chemistry and physics in the planet-forming zones of disks

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I

Introduction

Questions about our origin have always fascinated humankind. Where do we come from? How did life arise from the beginning? Is the origin of life something specific to our own planet? Indeed, can life exist elsewhere? Many of these questions will remain unanswered for many more generations to come and require progress in many small steps. In this thesis one of these smalls steps towards answering the question about the origin of life is taken by studying the regions around stars where terrestrial, hence Earth like, planets are thought to be forming. These are the planets that today we think would be the best candidates for having life supporting conditions.

1.1 The formation of planetary systems

The formation of a planetary system starts with the formation of substructures in molecular clouds that can contract under their own gravity. These parts of the molecular cloud get more and more dense until their cores reach such high densities that stars are born there (see reviews by Bergin & Tafalla 2007, di Francesco et al. 2007). Because of angular momentum, the collapsing core will rapidly form a circumstellar disk around the star. The most deeply embedded phase is called a class 0 object or protostar. The material from the collapsing envelope will start to accrete onto the star through the disk. The star in turn will heat up the surrounding disk and envelope. Some of the material will be ejected in the form of a stellar jet or disk wind along the rotational axis. This will disrupt and clear away the envelope. This phase of the still young protostar is called the class I stage, see Adams et al. (1987) and André et al. (1993) for further details on classification. Once most of the envelope has accreted onto the disk or been blown away by the wind, only the disk is left around the star. The disk is the location where planets are thought to be formed and is therefore called a protoplanetary disk. The object is a T Tauri star if the stellar mass is < 2 M_{Sun} and a Herbig AeBe star if the mass is within the range 2 – 8 $M_{\odot}$. The formation and evolution of the pre-main sequence star and a protoplanetary disk is summarised in Fig. 1.1. That these protoplanetary disks indeed exist in reality and not just in theory has been confirmed by the detection of an infrared access in their spectral energy distribution (SED) that could only be explained by a disk around the star (Kenyon & Hartmann 1987, Calvet et al. 1992, Chiang & Goldreich 1997, Men'shchikov & Henning 1997, D'Alessio et al. 1998). Later on direct observations done by for example the Hubble Space Telescope of circumstellar disks or proplyds, as they also can be called when an external light source illuminates them on the sky, could further prove their existence (see Fig 1.2) (O'Dell et al. 1993). In addition these disks can be detected by observing scattered stellar light on the dust grains located in the disk (Grady et al. 2005, Fukagawa et al. 2004, Clampin et al. 2003, Heap et al. 2000, Augereau et al. 2001, Grady et al. 1999).

In the early stages of the protoplanetary disk the temperature in the inner disk is hot enough so that all primordial grains are sublimated. Once the gas cools down, various compounds can start to condense. Which species condense out, and hence the chemical composition of the inner disk, will vary with the temperature and the cooling time which are both very dependent on the radial and vertical location of the gas. At this point, planets can start to form. The type of planets, their atmospheres and their radial location and their mass distribution will then strongly depend on the chemical and physical structure of the disk (see reviews by Prinn 1993, Ehrenfreund & Charnley 2000, Markwick & Charnley 2004, Bergin 2009). How this planet formation process proceeds and what will be its products can be better understood by studying the physical and chemical evolution models of the gas and dust in these disks. Fig. 1.3 shows an overview of typical chemical

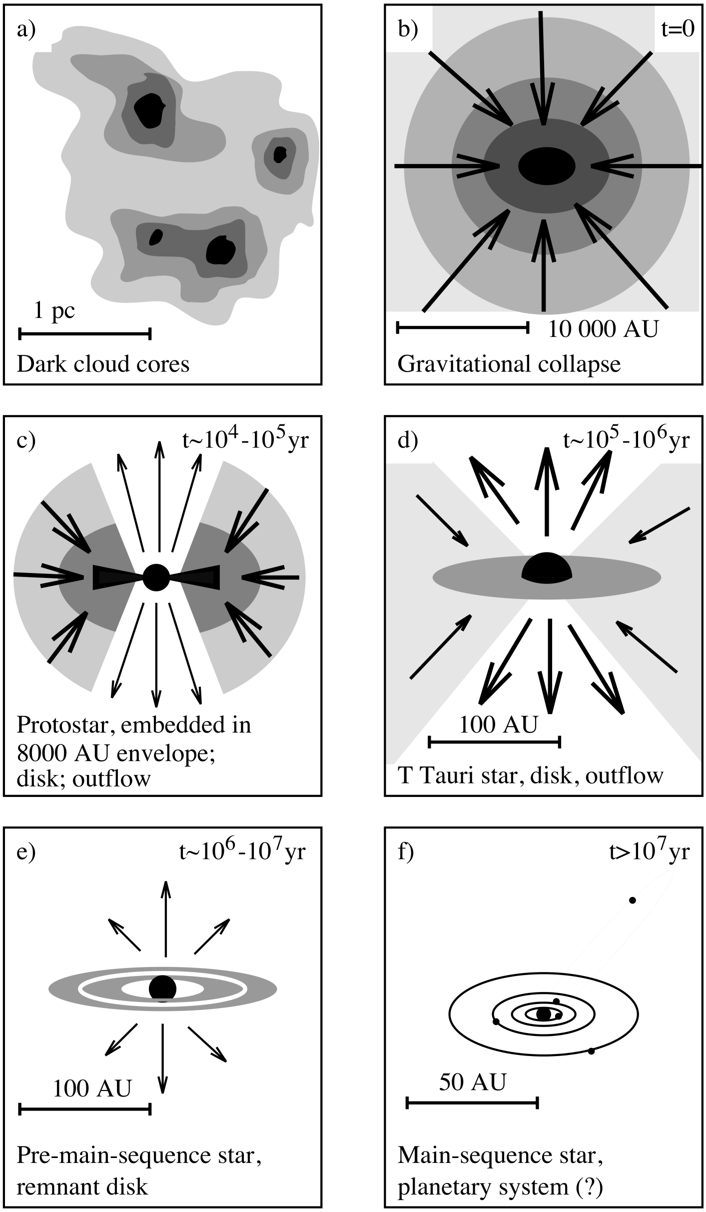

Figure 1.1 The formation and evolution of a protoplanetary disk. The different stages are shown, going from the dark cloud core, through the embedded proto star phase, with its circumstellar disk and outflow that carves out the envelope, until the protoplanetary disk becomes visible and a planetary system can form (Hogerheijde 1998).

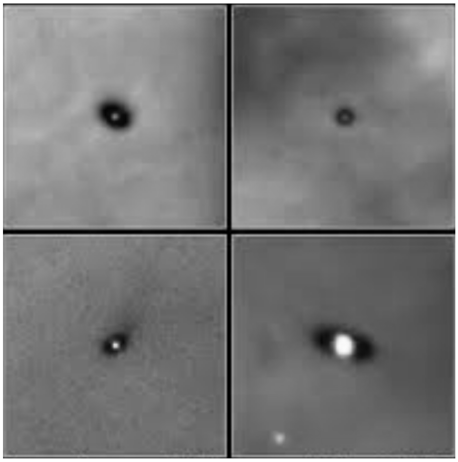

Figure 1.2 Direct observations of protoplanetary disks in the Orion nebula using the Hubble space telescope. Note how the disk is shown as a darker shadow surrounding the stars in front of the bright nebula. These protoplanetary disks have radii ranging from 100 – 300 AU (McCaughrean & O'Dell 1995, Bally et al. 2000).

conditions and physical processes in a protoplanetary disk.

The habitable zone of protoplanetary disks is especially interesting to study. This region is the zone in which a planet can have the proper conditions to be able to form or at least maintain life. One of the requirements is that the planet can have a temperature than permits liquid water on its surface. All life - as we know it - needs liquid water, so this is often considered a necessary condition for life. This habitable zone is in our own solar system estimated to be between 0.95 – 1.37 AU (Kasting et al. 1993). However, this radial range varies with different planetary and stellar properties. One factor is the luminosity of the star. For higher stellar luminosities, the habitable zone will move further away from the star and broaden. For example, the habitable zone is larger around F stars than around our Sun (a G star) and it is smaller around K and M stars.

Circumstellar chemical and physical evolution disk models start with initial conditions such as the temperature and density distribution and kinematics of the gas, chemical composition and gas/dust ratio of the disk. The chemical and physical structures that the models produce can then be compared with the observations of the gas and dust in protoplanetary disks (Natta et al. 2007, Bergin et al. 2007b). the next step is to compare with existing and future even more detailed observations of exoplanets and their atmosphere (e.g., Mayor & Queloz 1995, Borucki et al. 2011, Madhusudhan et al. 2011, Désert et al. 2011, Brogi et al. 2012).

1.2 A chemical and physical inventory of planet-forming zones

As discussed in Section 1.1 it is very important to understand the different physical and chemical properties of the protoplanetary disk to be able to understand how and which type of planets that form there. It is especially interesting to be able to define these properties in the inner regions of these disks since this is where the habitable zone is located. These parameters will not just help constraining the chemical evolution disk models but also the planet-formation models. These chemical disk models can then simulate and address the evolution of the organic inventory with characteristics such as temperature structure, different radiation fields and different molecular abundances.

It is for example interesting to study which types of more complex organic molecules can be constructed. It is observationally difficult to determine the inventory of large complex molecules as their abundance is expected to be low. Hence chemical models are required to predict abundances of complex molecules and these models have to be based upon observations of simple molecules. These more complex molecules are very interesting to study since they are considered to be the most important ones in being able to form planets with preferable conditions for life.

There are several different types of chemical evolution disk models. What mainly separate them are their different ways of breaking carbon out of CO and nitrogen out of N_2. The Najita et al. (2011) model for example include a X-ray field and the Agúndez et al. (2008), Woitke et al. (2009), Willacy & Woods (2009), Vasyunin et al. (2011), Walsh et al. (2012) models include an UV-field and photo-ionisation and photo-dissociation processes. The Walsh et al. (2012) model takes both the X-ray and UV-fields into account. There are also other important parameters such as cosmic ray ionisation, gas versus dust temperatures and the settling of the disk. Models also differ in the size of the chemical networks considered and the types of chemical reactions included. Molecular observations of protoplanetary disks can provide key tests of such models.

As circumstellar disks are small and not very luminous, good telescope and spectrometers with both very high spatial and spectral resolution are required in order to study chemistry and physical conditions in the inner regions of disks. The first observations of these sources were done at submillimeter and radio wavelengths since at these wavelengths high spectral and spatial resolution can be achieved by the use of single dish and interferometry. Molecules such as CO, H_2O, HCO^+, H_2CO, HCN, N_2H^+, CN, C_2H, SO, DCO^+ and DCN have been detected in this way (Dutrey et al. 1997, Kastner et al. 1997, Thi et al. 2004, Fuente et al. 2010, Henning et al. 2010, Öberg et al. 2011, Hogerheijde et al. 2011). However these observations cover the colder gas which is mainly located $>$ 100 AU in the disk which is not where most planets are thought to be forming. Only in the last 15 years have telescopes become sensitive enough to study the chemistry in the

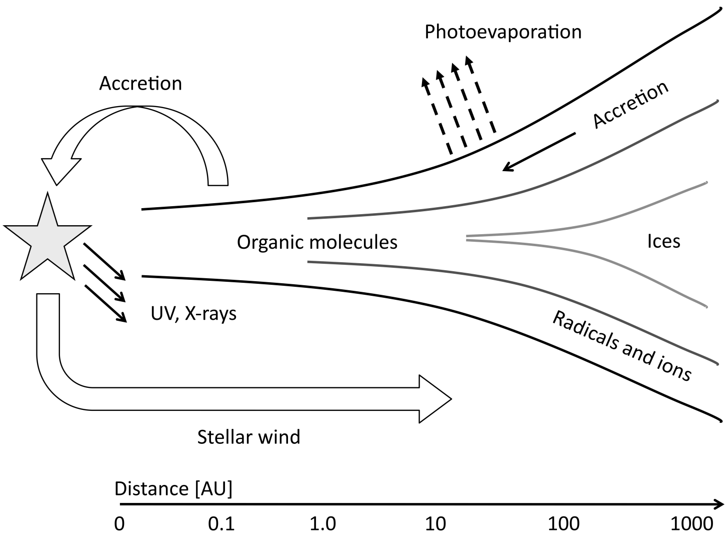

Figure 1.3 An overview of the different physical processes in a protoplanetary disk and its chemical structure; Material is accreted from the envelope and transported through the disk to the inner regions where accretion onto the star can occur. The gas gets photo-evaporated further out in the disk since the thermal speed of the gas can more easily exceed the escape velocity in these regions than in the inner disk (Störzer & Hollenbach 1999). Young stellar objects often have stellar winds which may impact the disk. Stellar UV and X-ray photons produce a photodissociation region on the surface of the disk. In the midplane there is ongoing ice accretion. Photo-desorption causes sublimation from ices in the surface layers of the disk. Warm chemistry in the inner regions (< a few AU) or in the surface layers produces more complex molecules at a few hundred up to a few thousand Kelvin.

inner regions (< 10 AU) of the circumstellar disks.

CO was the first molecule observed to originate from the hot inner disk (e.g., Najita et al. 2003, Brittain et al. 2003, 2007, 2009, Blake & Boogert 2004, Pontoppidan et al. 2008, Salyk et al. 2009, 2011b, Brown et al. subm.) and this was quickly followed by observations of H_2O, OH, CO_2, C_2H_2 and HCN (Carr et al. 2004, Lahuis et al. 2006, Gibb et al. 2007, Carr & Najita 2008, Salyk et al. 2008, Pascucci et al. 2009, Najita et al. 2010, Pontoppidan et al. 2010, Carr & Najita 2011, Kruger et al. 2011, Salyk et al. 2011). A very important milestone was the first detection of water (Carr & Najita 2008, Salyk et al. 2008) in these regions. This is because the presence of water is generally considered to be a necessary condition for life. Today we know that water and also other pre-biotic molecules such as HCN seem to be abundant in these regions and hence the warm gas in the planet forming zones of these disks seems to nourish a rich organic inventory. There are therefore many reasons to continue to gather even more information about these regions to be able to improve our knowledge about the physical and chemical conditions of these planet-forming zones.

1.2.1 Probing planet-forming regions with infrared observations

Near infrared and mid infrared observations around 1 – 30 μm are the best way to study the gas in the inner planet-forming zones of circumstellar disks. This is because the gas in these regions is warm, ranging from a few hundred to several thousand Kelvin, and therefore emits copiously in this wavelength region. In the near-infrared, around 1 – 5 μm, observations can be done from the ground and this allows the use of large spectrometers with high spectral and spatial resolution. Such instruments cannot be included in space-based observatories because of space and weight limitations. The best spectrometers today that can be used for observations within this wavelength range are NIRSPEC with a spectral resolving power of $R = \delta\lambda/\lambda = 25{,}000$ at the Keck telescope and the CRIRES spectrometer ($R = 10^5$) at the Very Large Telescope (VLT). This high spectral resolution means that the spectral lines can be individually resolved and even details of the line profiles can be detected. Most of the mid infrared lines from 5 – 30 μm cannot be observed on Earth because the atmosphere that is opaque at these wavelengths. The spectrometer IRS at the *Spitzer* Space Telescope is the instrument that has been primarily used within this wavelength range. Observations from all of these three telescopes are presented in this thesis. In particular, this thesis makes use of data from a large VLT-CRIRES program surveying ~70 disks around T Tauri and Herbig Ae stars (Pontoppidan et al. 2011b, Brown et al. subm.) For an overview of the various kinds of observations used for studying the emission from the relevant regions see Fig. 1.4.

The main focus of this thesis is to study emission and absorption lines from the

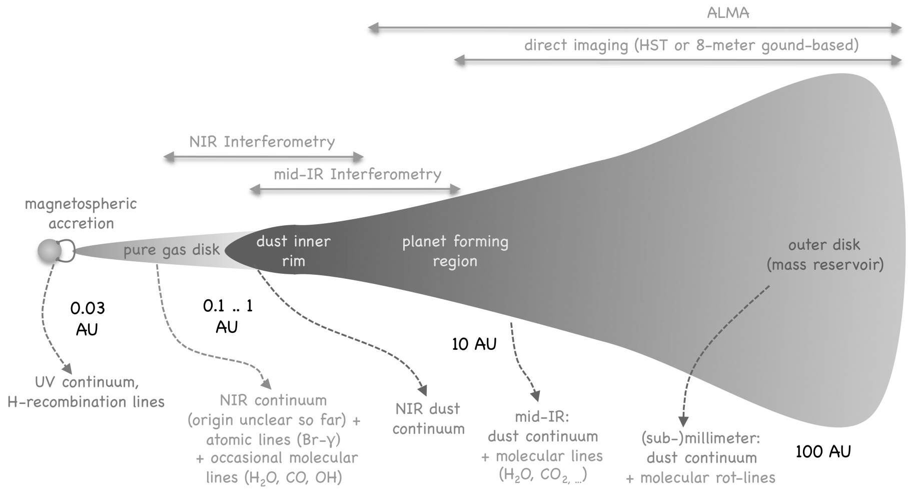

Figure 1.4 An overview of which areas of a protoplanetary disk different types of observations cover. In addition the type of continuum plus molecular emission that can be expected from different parts of the disk are presented here (Dullemond & Monnier 2010).

molecules H_2O, OH, CO_2, C_2H_2 and HCN. These molecules are all important prebiotic molecules and are also building blocks of more complex species. In addition, these molecules are sensitive tracers for the temperature and the different radiation fields in the disk. Their sensitivity as tracers means that by studying for example their relative and absolute amounts one can decide which the main reaction routes within a chemical network must have been to form them. These reaction routes are often controlled by an activation barrier that requires high temperatures to proceed. Reaction routes can also be affected by the local radiation field as that sets the level of ionisation and ions may react much more quickly than neutral species. These observations can also address evolutionary questions related to the origin of the relevant species. Specifically, are these molecules formed in the very early class 0 stage on the colder dust grains or later during the class II stage in the hot chemistry in the upper layers of the disk. It will also contribute to the more general astrochemical understanding of which type of chemical processes that play an important role in the formation/destruction reactions for different molecules in these environments.

In this thesis the focus is on ro-vibrational transitions of molecules. Unlike pure rotational transitions, which are predominantly emitted by cold gas far out in the disk, mid-IR ro-vibrational lines originate in the warm gas in the inner disks. These type of molecules can go through both vibrational and rotational transitions which do impact each other. This interaction is however so small that it can be omitted at a first order approximation when estimating the total ro-vibrational energy for one transition level. The total energy $E_{vib,rot}$ of a ro-vibrational transition can therefore be calculated using equation:

$$E_{vib,rot} = E_{vib} + E_{rot} = \left(v + \frac{1}{2}\right) h\nu_0 + hc\bar{B}J(J + 1) \tag{1.1}$$

where v is the vibrational quantum number, J is the rotational quantum number, h is Planck's constant, ν_0 is the frequency of the vibration, c is the speed of light, and $\bar{B}$ is the rotational constant. Due to quantum mechanical selection rules, only transitions where ΔJ is 0, ± 1 are allowed. The transitions will split out into R, Q and P-branches characterised by $\Delta J = 1$, 0 and -1 (see Fig 1.5). Note that some molecules (e.g.., CO) do not have a Q-branch e.g., $\Delta J = 0$ is not allowed. As an example the spectrum of the ν_3 mode of the C-H stretch at 3.019 μm of HCN has been plotted in the middle panel of Fig. 1.6 where the R, P and Q branches can be clearly seen. The overall extent of the P and R branches will depend on the level populations, in v=1 for emission and v=0 for absorption. These level populations are set by collisions - and hence are sensitive to the density and temperature of the emitting gas - as well as by the radiation field that can excite levels as well. Thus, the envelope of the P and the R branches will be broader for warmer gas, for denser gas and for gas that is pumped by a radiation field (see Fig. 1.6). The individual lines in the Q branch will generally blend into one broad feature. The profile of this feature will however still be set by the level populations and this can be used to derive the physical conditions in the emitting or absorbing gas.

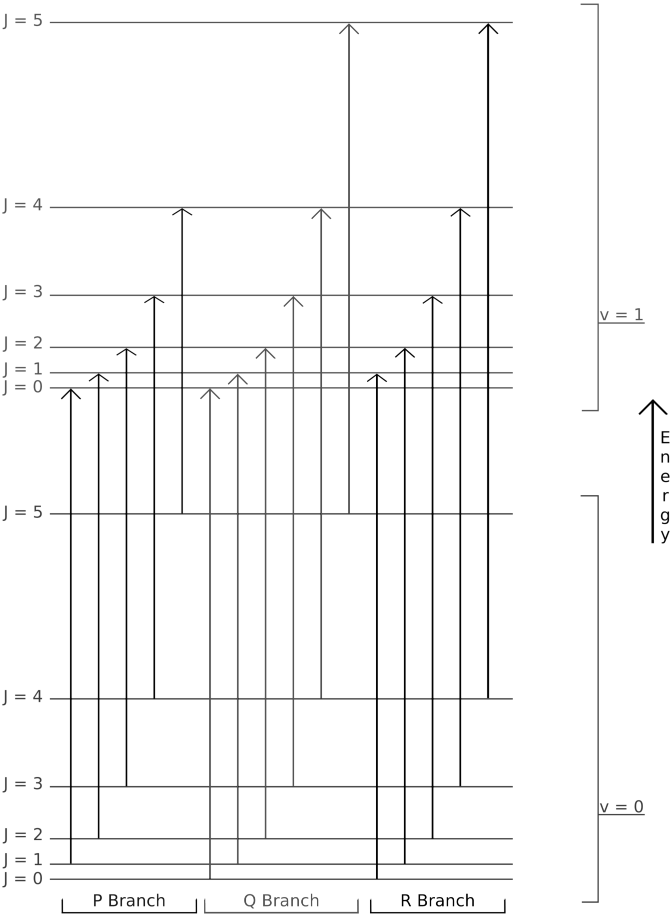

Figure 1.5 A schematic diagram of ro-vibrational transitions to illustrate how the R, Q and P branches arise.

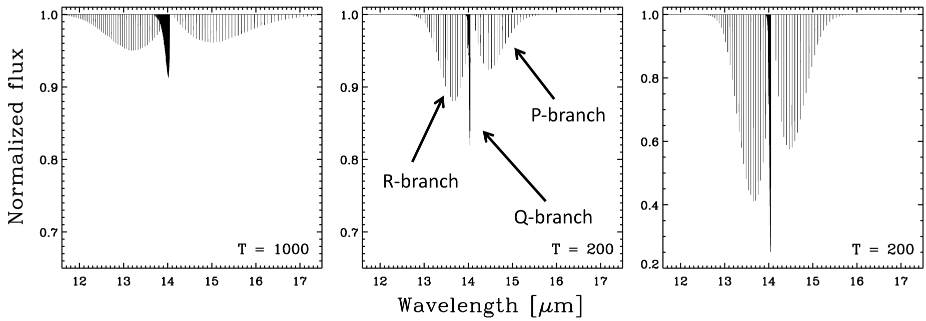

Figure 1.6 Absorption spectra of the ν_3 mode of HCN at the temperatures 200 and 1000 K and column densities $3.0 \cdot 10^{16}$ (left and middle panel) and $7.0 \cdot 10^{16}$ cm^{-2} (right panel).

1.3 This thesis

We now know that by studying the physical and chemical conditions in protoplanetary disks we can better understand how planetary systems are formed. These studies provide input for studies of planet-formation. They are what we can call the recipe for planets. However we also know that in order to use these models we need the parameters, hence the ingredients, for these recipes. The goal of this thesis is to provides these physical and chemical ingredients by using observations. The main questions together with short explanations for how we can use observations to answer these question are summarized here:

- **Which molecules can be found in these regions?** - Trying to detect different molecules by using observations.

- **What is the temperature of the gas where we detect the molecules?** - The comparison between the relative strengths of lines of a molecule provides a probe of the temperature of the gas where these molecules are excited.

- **Which type of excitation processes dominate?** By relating the observed excitation of these molecules to the local physical conditions (density, temperature, and radiation field), the dominant excitation process - collisions versus radiation - can be studied.

- **What is the spatial location of these molecules?** - The use of radiative transfer disk models can analyze line profiles of spectrally resolved lines to determine their spatial location. Different spatial distributions of a certain molecule will have different types of line profiles.

- **What are the chemical processes that form these molecules?** - By modeling the different intensities of the different molecular line profiles relative abundances can be estimated. These abundances can in turn be compared to the expected relative abundances that different chemical disk models predict depending on their different dominating chemical processes.

The four following chapters summarise the work that has been done addressing these questions. The main content of each chapter is described here:

Chapter 2: The origin of unexpected CO line profiles

During the investigation of CO emission line profiles, 8 out of ~50 T Tauri stars showed a broad based single peaked line profile. This type of line profile does not agree well with the expected line profile from Keplerian rotating gas in the inner region of a protoplanetary disk. An investigation was therefore done using the high spectral resolution CO 4.7 μm lines to see if the origin of these types of line profiles could be explained. The investigation showed that all of the 8 sources have in common that they have high mass accretion rates and have higher line to continuum ratios than their parent sample. In addition their CO lines are excited to higher vibrational states up to v = 2, and 4 out of 8 sources up to v = 4, and their rotational excitation temperature (~300 − 800 K) is lower than their vibrational temperature (~ 1700 K). This tells us that their CO lines are UV - pumped and hence exposed to a strong UV-field. The observations also show that the emission comes from within a few AU and has a velocity shift of < 5 km s^{-1} relative to the radial velocity of their parent star. One of the main results from this investigation is that these line profiles could not solely originate from a Keplerian rotating disk as was earlier expected. In addition an origin in a funnel flow and in magnetically, FUV or X - driven winds could also be ruled out. The results show that a combination of a disk plus a slow EUV launched disk wind is the most probable explanation of the birth place for these broad based single peaked line profiles.

Chapter 3: First detections of near infrared emission from organics

Only three molecules H_2O, OH and CO have previously been detected in near-infrared emission from the innermost regions of protoplanetary disks. The difficulty in detecting more molecules has to do with the large amount of the same molecules in the atmosphere of the Earth. The atmospheric molecules create very broad saturated absorption lines in the spectra that totally dominate the much weaker emission lines from the circumstellar disks. By observing the disks while they are having an as high as possible relative radial velocity shift to the Earth, combined with a very precise modeling of the atmospheric absorption lines, we are able to present the first detections of HCN near-infrared emission lines in 3/3 observed sources and C_2H_2 emission lines in one source as well as very stringent upper limits on both NH_3 and CH_4. Relative abundances of these molecules as well as of H_2O and OH are presented and their excitation temperatures are extracted by using both a radiative transfer slab model and a more precise disk model to compare the results with each other. Both models give comparable results. These 3 protoplanetary disks, which all belong to the same sample of the 8 disks discussed in Chapter 2 with single peaked broad based CO line profiles, also show the same type of line profiles for these organic molecules. Hence the origin of these organics may as well be linked to a disk + disk wind.

Chapter 4: Investigation of HCN excitation in protoplanetary disks

Earlier radiative transfer slab and disk models used local thermodynamic equilibrium (LTE) as an approximation in their models when trying to fit observed near- and mid-infrared line fluxes from the planet-forming zones of the disks. This approximation is done since implementing non-LTE in those models is a cumbersome and time consuming task. The main problem is however that the line emission from these regions is thought to come from gas that does not achieve high enough densities to be well described by LTE. A study is therefore presented in this chapter to investigate how the 3 and 14 μm emission from these regions will change using non-LTE in a slab model relative to LTE conditions and also to include radiative pumping in the excitation process of the HCN molecule. We conclude that the 3 μm line fluxes will be overestimated and hence the column density of HCN underestimated when using a LTE model. In addition it is shown that a slab model including both non-LTE and in addition radiative pumping will much better describe the excitation at 3 μm and hence derive better estimates of the HCN abundance. The 14 μm line emission is however not as much affected by non-LTE excitation since it reaches LTE at much lower densities than the 3 μm emission due to its lower critical density.

Chapter 5: Exploring organic chemistry in planet-forming zones

An investigation using high S/N *Spitzer* data was performed here for the first time to look for the most abundant more complex organic molecules in the inner regions of disks predicted by chemical models. This was done by studying two edge-on disks which show absorption lines instead of emission lines. Absorption lines have the main advantage that they have a much stronger line to continuum ratio compared to emission lines and hence much less abundant molecules can be studied. We have detected absorption lines of CO_2, HCN and C_2H_2. Analysis of the observations reveals similar abundances as observed for deeply embedded protostars as well as for comets in our own Solar system. This intriguing result suggests that (part of the) cometary material originates from the inner warm regions of the Solar Nebula. We also establish 3σ upper limits for the abundance ratios of C_2H_4, C_2H_6, C_6H_6, C_3H_4, C_4H_2, CH_3, HNC, HC_3N, CH_3CN, NH_3 and SO_2 relative to C_2H_2 and HCN. A comparison shows that the upper molecular limits relative to C_2H_2 and HCN agree much better with high temperature chemistry disk models including both UV and X-ray irradiation rather than just a X-ray irradiation. Also, the NH_3/HCN abundance tells us that the NH_3 molecules must have been formed in the warm chemistry of the disk atmospheres instead of being evaporated from the icy mantles of dust grains coming from the earlier stages of the disk evolution. In addition, simulations for future instruments like JWST, SOFIA, SPICA and ELTs show that molecules with at least one order of magnitude lower abundances relative to *Spitzer* observations can be detected with these future instruments. This would mean that much more strict constraints can be put on future chemical disk models.

1.4 Main conclusions

The main aim of this thesis is to contribute to the understanding of the physical and chemical conditions in regions of planet formation. This has been done by extracting physical and chemical parameters of the gas in the inner regions of protoplanetary disks by using infrared observations to better constrain planet formation and chemical disk evolution models. The extracted parameters and their resulting conclusions that could be drawn from this work are as follows:

- **Detections and molecular abundances:** HCN and C_2H_2 have been detected in the innermost disk (< 1 AU) and their relative column densities extracted using the high spectral resolution CRIRES data in combination with our newly developed observational tools. In addition strict upper limits on NH_3 and CH_4 were found using CRIRES and for the first time upper limits on the organics and sulfur bearing molecules C_2H_4, C_2H_6, C_6H_6, C_3H_4, C_4H_2, CH_3, HNC, HC_3N, CH_3CN, NH_3 and SO_2 have been made using the *Spitzer* telescope.

- **Temperatures:** Excitation temperatures and temperature structures have been estimated for CO, H_2O, OH, C_2H_2, HCN and CO_2 using both slab and disk radiative transfer models, modeling both emission and absorption line profiles.

- **Origin of emission:** Evidence has been found for a non-Keplerian origin from detected CO, H_2O and HCN emission lines. The origin of the emission is concluded to come from a disk + disk wind. We have shown that modeling of line profiles is important to be able to constrain the spatial distribution of the gas.

- **Excitation and chemistry:** We have shown that emission from the inner region of a protoplanetary disk is not well described using a LTE slab model. It is therefore very important to include non-LTE, radiative pumping and both UV irradiation and X-rays in future radiative transfer and chemical evolution disk models.

1.5 Future prospects and outlook

This thesis shows that, today, we can start to get detailed information about the chemical and physical structure of the planet-forming zones which was earlier only possible in the outer regions by using millimeter observations.

Instruments like CRIRES could for the first time provide us with details of the line profiles in these regions and reveal the importance of being able to describe these line profiles. This is and will be a very exciting challenge for future modelers. It is not enough any longer to just model the intensities and excitation temperatures of the lines and assume simple approximations such as a spatial distribution consisting of gas in Keplerian rotation around a star. Future radiative transfer models need to include a combination of origins of the gas, such as different types of disk winds, funnel flows and the disk itself. In addition different types of radiation fields, non-LTE excitation and the gas/dust ratio are very important to include to get more detailed information about the excitation processes of these molecules. Chemical disk evolution models also need to include different types of radiation fields and expand their chemical networks with even more molecules and their different types of formation and destruction routes both on dust grains and in the warm gas.

New and even more detailed observations is the only way to provide the modelers with the necessary information they need to be able to improve their models. Telescopes such as JWST, SOFIA, SPICA and ELTs will be able to both push the detection limits for the less abundant and more complex organic molecules and in addition give even more detailed line profile or spatial information. It is especially interesting to compare these results with the upcoming observations done by ALMA of the outer cooler regions in the disk. These comparisons will provide us with a much more complete picture of protoplanetary disks and their evolution. This information will in the end help us to understand how such a wide variety of planets can form and, at least in one case, provide such favourable conditions that even life itself could evolve there.