English summary

Stars are born when large clouds of dust and gas start to contract due to their own gravity (upper left panel of Fig. 6.4). The contraction leads to the formation of a central protostar surrounded by a large envelope of in-falling material (upper right panel of Fig. 6.4). During the contraction the cloud is rotating which leads to the formation of a disc. These discs of dust and gas surrounding young stars are called protoplanetary discs since this is where planets are expected to form (lower left panel of Fig. 6.4). In the current understanding of planet formation, micrometer sized dust grains are expected to grow via coagulation or instability to form kilometer sized planetesimals, leading via collisions to protoplanets with diameters of a few thousand kilometers.

![Figure 6.4](image)

Figure 6.4 – Overview of the various stages of star formation (Shu et al. 1987).

When a planet is present in a protoplanetary disc, dynamical effects are expected to lead to the gradual removal of material from the orbit of the planet causing holes or gaps in the disc material. However, there are also other causes of gap/hole formation, such as grain growth and photo-evaporation. Photo-evaporation removes small dust and gas simultaneously, while grain growth removes only dust (the gas might be indirectly affected due to the changes of the dust). In the case of planet formation it is yet unclear whether the gas in the disc follows the dust in the removal process or if it remains in the dust holes. Hence, gas observations that can clarify the content/geometry of the gas in regions with dust cavities (e.g. near infrared spectra of the ro-vibrational transitions of the carbon monoxide molecule) can be very instructive for our further understanding of the presence of gaps/holes and its relation to planet formation.

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2 Photo-evaporation is a process where a molecule or particle, due to added energy from a photon, reaches the escape velocity of the system and "evaporates" into space.
In protoplanetary discs, temperatures and densities cover very large ranges of values. In the inner disc close to the star, the material is hot and dense (>1000 K and >10^{14} \text{ cm}^{-2}). Far away from the star in the outer disc, the material is colder and more sparse (<50 K and <10^{4} \text{ cm}^{-2}). Molecules or atoms in the disc can due to added energy (radiation) from the star become excited to a higher energy state. This excess energy is then re-emitted by the molecule and can be observed as molecular emission lines at a certain wavelength set by the energy of the transition. Different molecular transitions have different energies and transition probabilities which allows them to be linked to a certain area in the disc. This means that by observing different molecules, we see emission from different disc regions.

In this thesis I study the ro-vibrational transitions emitted by the CO (carbon monoxide) molecule, the second most abundant molecule in the universe. The ro-vibrational emission lines of CO are emitted from the regions of the discs where we typically expect to find gaps or holes due to planet formation, and could thus help to clarify the gas content/geometry in these regions.

In theory, emission lines in a spectrum are seen as simple, narrow, unextended
lines at the characteristic wavelength of the emitting atom or molecule. When the emitting object is moving, the line is shifted to another wavelength due to the doppler effect. When emission is coming from an inclined rotating disc, parts of the emitting material are moving towards us while other parts are moving away from us (if the disc is not inclined but viewed face on, the material has no velocity toward or away from the observer, relative to the central star). Due to the many different velocities seen in a rotating inclined disc, the emission is not seen as one line present at one wavelength, but instead spread out over a range of wavelengths and thereby broadened. These shifts in wavelength can be translated to velocities in the disc using the Doppler equation. Fig. 6.5 shows a sketch linking various locations in a rotating inclined disc to contributions in an observed line profile (for comparison, this is also shown for a face on disc). Since the velocity of the rotating material in the disc depends on its distance to the star, the width and the general appearance of line profiles can be used to infer the location in the disc where the lines are emitted. Hence, the detailed study of gas emission line profile shapes might yield important information on the geometry of the emitting gas. This can be compared to dust observations or used on its own to infer the presence (or lack) of holes/gaps possibly linked to planet formation.

Using high resolution observations of protoplanetary discs and detailed computer models, describing the physical conditions in the disc, its chemical composition and its geometry, I have explored to what extent the shapes of these emission lines can reveal the presence of holes or gaps in the inner regions of observed protoplanetary discs. If well understood, this could add additional pieces to the puzzle of how planets form.

In chapter 2, I compared modelled and observed CO ro-vibrational lines from a well studied disc of known geometry, HD 100546. This allowed me to test the disc model and develop the techniques used throughout the thesis. I also identified and exemplified slit loss effects for the first time. These effects are relevant for nearby protoplanetary discs observed through a narrow slit (typically used when observing CO ro-vibrational lines). These purely observational effects can create similar line profile variations as seen by physical effects such as disc winds, outflows or disturbances in the gas dynamics due to planets.

In chapter 3, I studied CO ro-vibrational lines from a sample of observed discs. Taking these new observations together with CO ro-vibrational lines from previous observed protoplanetary discs in the literature, I sought to draw general conclusions about the measurable quantities of CO ro-vibrational emission. Two opposing behaviours were identified for the different studied objects: 1) All CO ro-vibrational lines from one disc have the same width. 2) Lines from one disc become gradually broader for lines of higher excitation energies. The constant behaviour might be related to the presence of a gap in the disc which confines all lines to one similar limited emitting region and an increasing width might be linked to discs without any gaps. In a handful of observed sources, the CO ro-vibrational emission lines indicate that gas is present close to the star, while dust observations indicate that a dust gap or hole is present in these inner regions.
This suggests that gas can sometimes remain in a region where the dust has been removed.

In chapter 4, I compared modelled and observed CO ro-vibrational lines from another well studied disc of known geometry, HD163296. In this case, CO ro-vibrational emission lines observed with a different instrument collected 10 years earlier were added to the study. The comparison with the previous data revealed that the CO ro-vibrational line profiles have changed over time and our analysis points to an additional component of emission not coming from the rotating disc but possibly from the root of a molecular outflow. In this chapter, I also tested a frequently used analytical method to infer gas temperatures: The fitting of the slope of Boltzmann diagrams. In cases with large error bars or when the emission is coming from an extended region with different temperatures, the temperature estimates from this method were found to be often unreliable.

In chapter 5, I created a grid of 20 disc models (Fig. 6.6 shows sketches of selected models) with differing geometry, e.g. large dust holes (model A7), small dust holes (model A6), dust gaps (model A8), or no gaps/holes (model #0), to address what changes this induces in the line profiles. From this model grid, I derived several general trends that can be used as independent geometry indicators in future studies of CO ro-vibrational lines from protoplanetary discs, not only for the gas, but also to some extent for the dust.

To summarise, observations of CO ro-vibrational fundamental emission lines can provide crucial information on the location of gaps both in the gas and in the dust of protoplanetary discs. Inner disc geometries that can appear degenerate from dust observations alone, could be separated by analysing CO ro-vibrational line profiles. In almost all cases of CO ro-vibrational lines, the high resolution instrument CRIRES (CRyogenic high-resolution InfraRed Echelle Spectrograph) on the VLT (Very Large Telescope) could (with high signal to noise) fully resolve the detailed shapes of these lines. CRIRES/VLT is not currently available and the second best resolution offered at this wavelength is from NIRSPEC (Near-Infrared Spectrograph) on the Keck telescope. The somewhat lower resolution that this instrument offers means that some details in line shapes can be lost. Hence, for future detailed studies of CO ro-vibrational line profiles the availability of an instrument with a spectral resolution comparable to the CRIRES/VLT is vital.
Figure 6.6 – Sketch showing the gas and dust geometry of selected models from the modelling grid. Model #0 - the base model, A6 - large dust hole, A7 - small dust hole, A8 - dust gap, B3 - large dust and gas hole, C4 - flat disc, AC2 - flat disc with large dust hole.