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High angular resolution studies of protoplanetary discs

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CHAPTER 7

Abundant warm molecular gas in the disc around HD 100546

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THE disc around Ae star HD 100546 is one of the most extensively studied discs in the southern sky. Although there is a wealth of information about its dust content and composition, not much is known about its gas and large scale kinematics. Many recent results have stressed the importance of studying both the gas and dust in discs. ^{12}CO is an excellent gas tracer in the submillimetre, and the ratio between the lines of low and high rotational levels probes the gas temperature. Emerging submillimetre facilities in the Southern hemisphere allow us to characterise the gas and dust content in objects like HD 100546 better. We observe the molecular gas toward HD 100546 using the Atacama Pathfinder Experiment telescope. The lines $^{12}\text{CO } J=7-6$, $J=6-5$, $J=3-2$, $^{13}\text{CO } J=3-2$ and $[\text{C I}] ^3\text{P}_2-^3\text{P}_1$ are observed, diagnostic of the warm disc surface layers, disc size, chemistry, and kinematics. We use parametric disc models that reproduce the low- J ^{12}CO emission from Herbig Ae stars well. With the help of a molecular excitation and radiative transfer code we fit the observed spectral line profiles. We find that $\approx 0.01 M_{\odot}$ of molecular gas is present within 400 AU from the star, based on the observed optically thick ^{12}CO lines, consistent with the dust continuum fluxes in the literature. The lines arise from gas at 20-60 K. The puzzling non-detection of the $[\text{C I}]$ line indicates excess UV emission above that of the stellar photosphere. Asymmetry in the ^{12}CO line emission suggests that one side of the disc is slightly colder than the other. A plausible scenario is an asymmetry in the structure of the inner 200 AU of the disc, affecting the heating of the outer disc. We also consider pointing offsets and asymmetry in the disc extent as possible, but unlikely scenarios. We exclude foreground or extended emission as a cause of the observed line asymmetry.

7.1 INTRODUCTION

Over the past decade our understanding of the structural and physical properties of discs around young stars has increased from basic theoretical modeling of the spectral energy distributions (SEDs) constrained by observations with no spatial information, to modelling based on not only the SEDs, but also spatially resolved dust observations, like scattered light images and interferometry (Pinte et al. 2008; Tannirkulam et al. 2008, and Chapter 3 of this thesis). Two decades ago, the first submillimetre interferometer observations resolved the molecular gas emission spatially and this allowed major progress in understanding the disc kinematics, structure and chemistry (see Beckwith & Sargent 1987; Koerner et al. 1993; Dutrey et al. 1994, and later work by those authors). (Sub)millimetre gas and dust emission is the ideal probe of the global disc properties, like size, mass and radial distribution of disc material, because the bulk of the disc mass is located beyond 100 AU from the star and at temperatures of only 10-50 K that dominate this part of the spectrum. Recently, disc modelling including constraints of both dust and molecular gas observations has stressed the importance of analysing the gas and dust components simultaneously, in the context of each other (e.g. Wilner et al. 2003), as done in Chapters 2 and 3 of this thesis.

Until recently, observations of rotational transitions of molecules in the submillimetre regime were focused primarily on low- J emission from ^{12}CO , up to the $J=3-2$ line (Greaves et al. 2000; Thi et al. 2001; Qi et al. 2004; Thi et al. 2004; Dent et al. 2005a). In two of the brightest and most studied sources, TW Hya and LkCa 15, the observations of higher- J transitions of ^{12}CO were compared to the low- J lines, providing indications of the gas temperature in the intermediate-height molecular layer (van Zadelhoff et al. 2001). The physical conditions in this layer are crucial ingredients for chemical modeling of discs. In van Zadelhoff et al. (2001) single-dish line spectra are fitted using simplistic disc models. They derive a temperature of 20-40 K in the ^{12}CO line-emitting layers of LkCa 15, and more than 40 K in TW Hya. Qi et al. (2006) analysed submillimetric interferometer observations of TW Hya in the context of a disc structure based on the accretion disc model of Calvet et al. (2002) and showed that X-ray heating of the gas is efficient in this source, in addition to the stellar radiation field. Such diagnostics of gas heating and ionisation improve our understanding of how the gas content evolves in discs.

The emerging millimetre facilities in the Southern hemisphere like the Australia Telescope Compact Array (ATCA) and the Atacama Pathfinder EXperiment (APEX) are opening the window towards the star-forming regions of the Southern sky and are well suited to study the circumstellar discs in these regions. These instruments also pave the path for future observations with the Atacama Large Millimeter / Submillimeter Array (ALMA), which will drastically improve our knowledge of disc structure and evolution. We use the APEX receivers APEX-2a and CHAMP⁺ to observe the ^{12}CO $J=7-6$, $J=6-5$, $J=3-2$, ^{13}CO $J=3-2$ and [C I] $^3\text{P}_2-^3\text{P}_1$ line emission towards the disc around the young intermediate-mass star HD 100546. A wealth of observations of dust in this bright disc (Waelkens et al. 1996; Malfait et al. 1998; Grady et al.

¹CHAMP+ was constructed with funds from NWO grant 600.063.310.10.

2001; Augereau et al. 2001; Bouwman et al. 2003; Acke & van den Ancker 2006; Ardila et al. 2007) has motivated us to probe its molecular gas content and kinematics. The chosen transitions are particularly sensitive to the gas in the warm upper layers and kinematics of the outer disc. Our millimetre line observations probe the outer radius and inclination. The existing observational constraints on these parameters in the disc around HD 100546 provide an excellent basis for the analysis of our data.

HD 100546 is a young B9V type, $2.5 M_{\odot}$ star, classified as a Herbig Be star due to its isolation, infrared excess and silicate emission (The et al. 1994; Malfait et al. 1998). With a distance of 103 ± 6 pc, measured by Hipparcos, this is one of the nearest Herbig Ae/Be stars. In van den Ancker et al. (1998) the age of the star greater than 10 Myr is estimated. This makes the presence of circumstellar material intriguing, considering that the disc is expected to dissipate within 10 Myr in most young stars (e.g. Hollenbach et al. 2000; Hernández et al. 2007). Based on SED modeling, Bouwman et al. (2003) postulate the presence of an inner hole in the disk of 10 AU radius, likely caused by a Jupiter-sized planet (see also Acke & van den Ancker 2006). Direct evidence of cold disc material at larger radii is provided by Australia Telescope Compact Array observations of Wilner et al. (2003) at 89 GHz (3.4 mm) and $2''$ resolution, with a flux of 36 ± 3 mJy, values consistent with the 1.3 mm observations of Henning et al. (1998). They do not detect HCO^+ $J=1-0$ line emission and speculate that photodissociation of CO in the upper disc layers or an overall gas depletion may be the reason for this. In the recent spectroastrometric observations of rovibrational ^{12}CO transitions, van der Plas et al. (2009) suggest that ^{12}CO is depleted from the inner disc regions (up to 30 AU from the star).

Scattered light imaging of HD 100546 reveals the disc extending up to $4''$ from the star viewed at an inclination of 50° , and an interesting disc structure resembling spiral arms (Pantin et al. 2000; Augereau et al. 2001; Grady et al. 2001). This structure was interpreted as due to disc perturbation by a companion (Quillen et al. 2005) and by a warped disc structure (Quillen 2006). Coronagraphic imaging by Augereau et al. (2001) finds steep surface brightness profiles in the environment of HD 100546 indicative of optically thin emission in the near-infrared, suggesting surface densities as low as $10^{-3} \text{ g cm}^{-2}$. Their images trace the emission of small dust ($< 5 \mu\text{m}$), extending out to 800 AU from the star. The authors suggest the presence of an optically thick disc and an optically thin flattened halo or envelope.

In Sect. 7.2 we present our observations of the ^{12}CO , ^{13}CO , and [C I] lines. All ^{12}CO and ^{13}CO lines are detected while the [C I] remains undetected, and we model the lines in Sect. 7.3 deriving disc gas temperatures.

7.2 OBSERVATIONS AND RESULTS

The observations of ^{12}CO $J=6-5$ at 691.472 GHz and [C I] $^3\text{P}_2-^3\text{P}_1$ ([C I] $J=2-1$ hereafter) at 809.344 GHz towards HD 100546 at $11^{\text{h}}33^{\text{m}}25^{\text{s}}.4$ and $\text{Dec} = -70^\circ 11' 41''$ (J2000) were obtained simultaneously with the CHAMP⁺ heterodyne array receiver (Güsten et al. 2008) on APEX on 2008 November 11. The 7 pixels in each wavelength band are arranged in a hexagon of 6 pixels around one central pixel pointed towards the source,

Line	I (K km s ⁻¹)	$FWHM$ (km s ⁻¹)
¹² CO $J=7-6$	12.2±1.9	4.2
¹² CO $J=6-5$	10.5±0.9	4.2
¹² CO $J=3-2$	4.0±0.6	4.0
¹³ CO $J=3-2$	1.3±0.6	–
[C I] $J=2-1$	<1.5	–

Table 7.1: Observed ¹²CO $J=6-5$ and $J=3-2$ line integrated line intensities, $I = \int T_{mb} dv$, and line widths $FWHM$. The upper limit on the [C I] line is a 2σ value.

with beam sizes of 9'' at 690 GHz and 7.7'' at 810 GHz. The data were obtained in a staring mode with a chop of 120''. The backend consisting of Fast Fourier Transform Spectrometer units on all pixels was used, providing a spectral resolution of 0.12 MHz or 0.05 km s⁻¹ at these frequencies. Main beam efficiencies are 0.56 at 690 GHz and 0.43 at 810 GHz. The calibration is uncertain by $\approx 30\%$ at both frequencies. Pointing was performed directly prior to the observations providing an accuracy better than 3''. The CO $J=6-5$ line was also observed on 2008 November 10 in jiggle mode and its intensity and spectral profile were found to be the same within 20%. During this observation, the high band was tuned to ¹²CO $J=7-6$ at 806.665 GHz. The ¹²CO $J=6-5$ data taken on 2008 November 11 are used in the further analysis.

The ¹²CO and ¹³CO $J=3-2$ lines at 345.796 GHz and 330.588 GHz, respectively, were observed on 2005 July 27 and 28 with the APEX-2a receiver using a single pointing. The spectral resolution of these data is 61 kHz or 0.05 km s⁻¹. The beam size and efficiency of APEX at 346 GHz are 14'' and 0.73, respectively. Our ¹²CO $J=3-2$ line data was presented in Chapter 5 of this thesis.

We have detected all the observed molecular line transitions, with exception of the [C I] $J=2-1$ line. Figure 7.1 shows the observed spectra, baseline subtracted, corrected for the beam efficiency and re-binned to a lower spectral resolution. The ¹²CO $J=3-2$ and $J=6-5$ lines are detected at the highest signal to noise ratio, and show a double peaked profile characteristic of disc rotation. The intensities integrated over the velocity range 0–10 km s⁻¹, over which line emission is detected, are listed in Table 7.1 together with the full width at half-maximum of the lines with sufficiently well defined profiles.

In addition to the observations towards the source, the CHAMP⁺ array provides measurements at nearby offsets. This setup provides an excellent way to discern the emission from the disc, with an estimated size of 400 AU in radius (Augereau et al. 2001), from the surrounding material known to be present further away from the star. The central pixel of our CHAMP⁺ data probes the ¹²CO $J=6-5$ line emission from the region of 9'' centered on the position of the star (450 AU radius), while the surrounding pixels probe the more distant regions (roughly 1000–2000 AU). Similarly, at the frequency of the ¹²CO $J=7-6$ line a smaller region around the star of 7.7'' is probed with the central pixel (390 AU radius), and regions roughly 1000–2000 AU with the surrounding pixels. Table 7.2 provides an overview of the pixel positions and the cor-

$^{12}\text{CO } J=6-5$ 9'' beam			$^{12}\text{CO } J=7-6$ 7.7'' beam		
RA offset (")	Dec offset (")	$I_{\text{CO}(6-5)}$ (K km s $^{-1}$)	RA offset (")	Dec offset (")	$I_{\text{CO}(7-6)}$ (K km s $^{-1}$)
-9.8	-17.0	0.4 ± 0.2	+10.2	-17.0	< 2.0
+8.8	-18.0	0.5 ± 0.2	+20.2	-1.4	< 2.0
-18.9	-0.2	< 0.2	-9.0	-16.5	< 2.0
+19.4	-1.2	< 0.2	+11.0	+16.2	< 2.0
-9.3	+16.6	< 0.2	-18.8	+0.2	< 2.0
+10.0	+16.6	< 0.2	-9.1	+16.9	< 2.0

Table 7.2: Observed $^{12}\text{CO } J=6-5$ and $J=7-6$ intensities integrated over a velocity range of 0–10 km s $^{-1}$, for each pixel of the CHAMP $^+$ heterodyne array.

responding fluxes integrated from a velocity range from 0 to 10 km s $^{-1}$, over which the ^{12}CO lines are firmly detected in the central pixel. Compared to the on-source fluxes, these measurements clearly show that the ^{12}CO emission from the surrounding material is about 20 times weaker than from the region within 400 AU from the star.

The $^{12}\text{CO } J=3-2$ line was observed with a single pointing of the beam of 14'', large enough to include any emission from regions beyond 400 AU. However, the strong resemblance in the line profile suggests that both low- J and high- J lines arise from the disc and that any contribution to the line emission by an extended low-temperature and low-velocity component is negligible. An extended envelope around HD 100546 extending to radii of 800 AU has been suggested based on optical imaging by Grady et al. (2001). However, considering the low dust density in the envelope, photodissociation of the molecular gas is expected to be efficient, resulting in largely atomic gas that does not contribute significantly to the ^{12}CO line flux. Considering this, it is puzzling that [C I] line emission is not detected in any of the CHAMP $^+$ beams.

Our data clearly show presence of warm molecular gas in the region extending up to several hundred AU from the star (450 AU for the 6–5 line and 700 AU for the 3–2 line). We obtain the following integrated intensity ratios, corrected for beam dilution: ^{12}CO lines (6–5)/(3–2)= 1.0 ± 0.2 and $(^{12}\text{CO } 3-2)/(^{13}\text{CO } 3-2)=2.8 \pm 0.5$.

There is a clear asymmetry in the profile of the ^{12}CO lines, observed at a high signal-to-noise ratio. In some sources, asymmetries like this are explained through confusion with cloud emission, as seen in ^{12}CO lines towards IM Lup (van Kempen et al. 2007) and DL Tau (Simon et al. 2000). Also, such asymmetry is seen in ^{12}CO lines from sources with a pronounced disc asymmetry, like HD 141569 (Dent et al. 2005b). Another possibility is a pointing offset along the disc major axis. In the following section we investigate these and other possible causes of the observed line asymmetry.

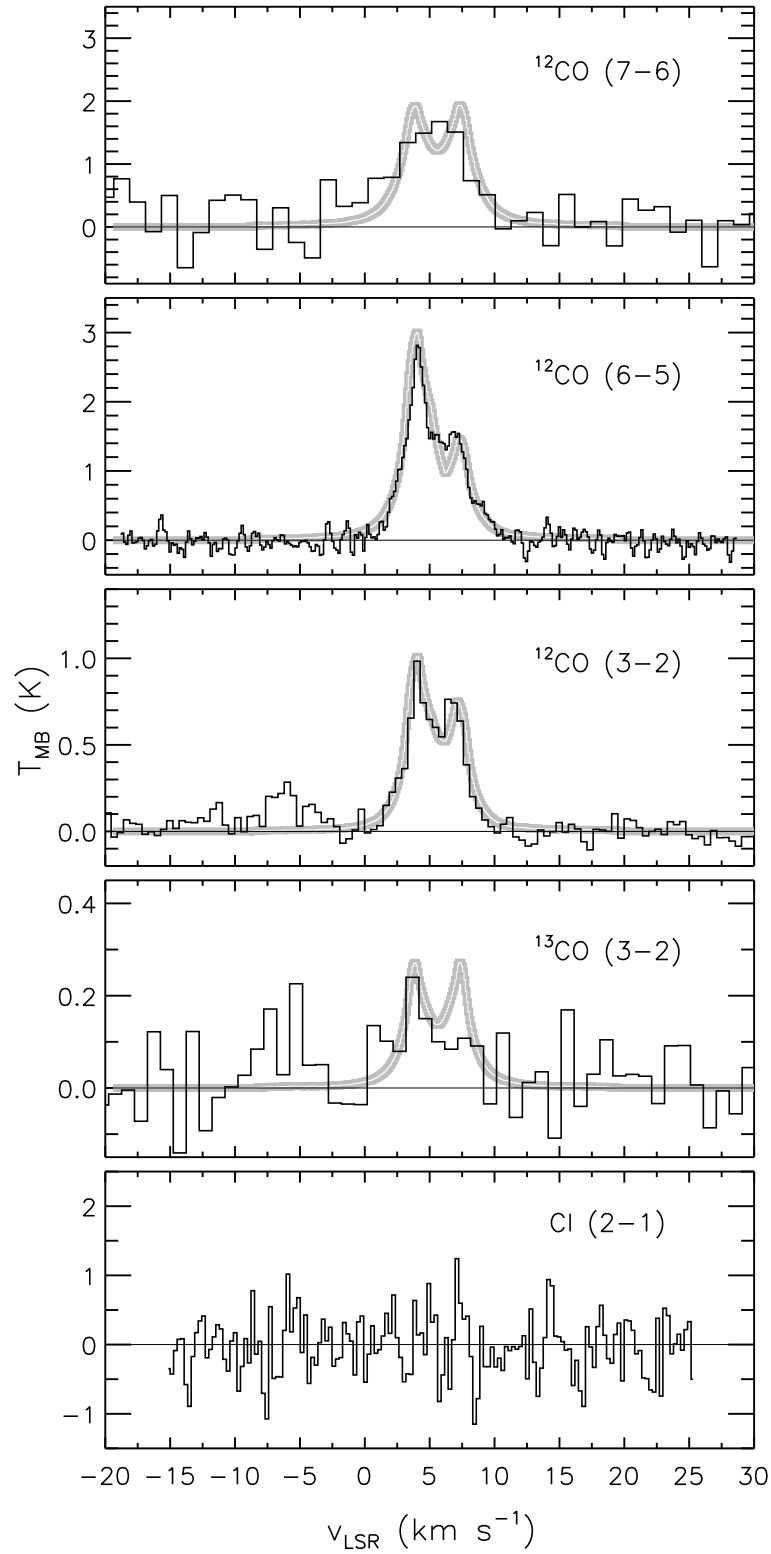


Figure 7.1: Spectra of the ^{12}CO and ^{13}CO submillimetre lines observed towards HD 100546, compared to our best fit models.

7.3 DISCUSSION

7.3.1 CO line emission

The ^{12}CO $J=3-2$ and $J=6-5$ line emission from circumstellar discs is generally optically thick and arises from warm upper disc layers. These lines are particularly sensitive to the temperature of these layers, and therefore to the stellar and external illumination of disc surface. The line ratio of $(^{12}\text{CO } 3-2)/(^{13}\text{CO } 3-2)=2.8\pm0.5$ indicates that the ^{12}CO line emission is optically thick and thus that substantial amounts of molecular gas are present in the disc around HD 100546. Assuming a temperature of 20 K, densities of $10^6\text{--}10^8\text{ cm}^{-3}$, and a CO/H_2 abundance of 10^{-4} , a column density of H_2 of roughly 10^{22} cm^{-2} reproduces the observed line ratio (calculation done with the RADEX online tool²). This column density is typical of outer regions of gas-rich discs. The low ^{13}CO line flux may be in part due to freeze-out and/or selective photodissociation. Detailed modelling and spatially resolved submillimetre line observations of ^{12}CO and isotopologues would allow to constrain the disc structure better, and evaluate the effect of these processes (See Chapter 2 of this thesis).

The line emission of $^{13}\text{CO } J=3-2$ is less optically thick than ^{12}CO , tracing deeper into the colder disc layers. A deeper integration of this line resulting in a higher signal-to-noise ratio would provide a better defined spectral profile. Comparison to the ^{12}CO line profile would allow us to draw conclusions on the relative spatial extent of the emission region of the two molecules and enable a more detailed modelling, including a disc vertical temperature structure and simple processes like freeze-out in the cold outer regions below disc surface layers (cf. Dartois et al. 2003).

Submillimetre ^{12}CO line emission is analysed using two different modelling approaches in the literature. Disc physical models, like the irradiated accretion disc models of D'Alessio et al. (2005), are especially well suited when the emission is spatially resolved and the three-dimensional structure of the disc can be investigated, for example when transitions of different optical depths are observed (Chapter 2 of this thesis). For spatially unresolved observations, like those presented here, simplistic models with a limited number of free parameters are more appropriate to derive some basic constraints on disc properties based on the line spectrum (Dutrey et al. 1994; Guilloteau & Dutrey 1998).

7.3.2 Disc parametric model and best-fit parameters

In Chapter 5 of this thesis, we show that simple power-law disc models, with a disc mass $M = 0.01 M_{\odot}$, surface density $\Sigma \propto R^{-1}$ and temperature $T = 60\text{ K } (R/100\text{ AU})^{-0.5}$, are useful tools to analyse low- J ^{12}CO transitions from gas-rich discs around Herbig Ae stars. We use these models to fit the ^{12}CO spectra. We fix the outer radius and inclination to the observationally constrained values of 400 AU and 50° (Augereau et al. 2001). The size estimate is based on the scattered light observations and is used as guidance

²<http://www.strw.leidenuniv.nl/~moldata/radex.html>

for molecular line modeling. Without sufficient amounts of gas the dust settles to the midplane, and the disc becomes self-shadowed. As the scattered light only probes the illuminated disc surface at some height above the midplane, it provides a lower limit to the actual size of the disc. The inner radius is assumed to be 0.6 AU, close to the dust sublimation radius. Although an inner hole of 13 AU is found in HD 100546, its presence does not affect our results because the molecular lines observed are dominated by the outer disc regions, far beyond inner tens of AU. The surface density is given by a powerlaw $\Sigma \propto R^{-1}$, and the temperature $T = T_{100} (R/100 \text{ AU})^{0.5}$, where T_{100} is a free parameter. The disc models are vertically isothermal, and the vertical density structure is calculated assuming hydrostatic equilibrium. The ^{12}CO abundance with respect to H_2 is assumed to be 10^{-4} , constant throughout the disc. Because the observed ^{12}CO lines trace warm molecular material and are insensitive to the colder regions deeper in the disc, it is reasonable to neglect freeze-out in these calculations.

For the estimated disc mass and observed $^{12}\text{CO}/^{13}\text{CO}$ line ratio, the observed ^{12}CO lines are optically thick, with a H_2 surface density of 10^{22} cm^{-2} . The evident line asymmetry mentioned in Sect. 7.2 cannot be fit by assuming different densities at the two sides of the disc, because the optically thick ^{12}CO lines are insensitive to the column density.

For the optically thick ^{12}CO lines, the temperature and the outer radius determine the line intensity, and any asymmetry in either of these two parameters affects the emerging line profile. We consider these two possibilities separately.

^{12}CO $J=6-5$ and $J=3-2$ line profile fit

Temperature asymmetry. In this scenario we consider that the observed line asymmetry is caused by a temperature asymmetry in the disc, with one side of the disc colder than the other. We use different T_{100} parameters for the two sides of the discs, separated by the minor axis. These two sides contribute almost exclusively to the two respective sides of the spectral line (with respect to the line centre at 5.6 km s^{-1}). The radial density structure is determined by our assumed disc mass, outer radius and surface density power-law. Some difference in the disc vertical thickness may be present as a result of different temperatures at the two sides, but this difference is negligible and the resulting spectra are insensitive to it.

We use the molecular excitation and radiative transfer code RATRAN (Hogerheijde & van der Tak 2000) to calculate the line emission from the model. In these calculations, Keplerian rotation of the disc around a $2.5 M_{\odot}$ star and a disc inclination of 50° (0° corresponding to face-on) are assumed. Dust continuum emission, although negligible for the molecular line transfer, is included in the calculation and subtracted from the final image cubes. The calculated emission is convolved with the corresponding beam size, and the spectra toward the image centre extracted.

We obtain the best fit to the ^{12}CO $J=6-5$ spectrum by assuming values of T_{100} of 40 and 60 K for the two disc sides, respectively. The ^{12}CO $J=3-2$ spectrum is fitted assuming 40 and 50 K, where the difference in temperature contrast may be explained by (part of) the ^{12}CO $3-2$ emission originating from deeper layers in the disc. The corresponding synthetic spectra are compared to the observations in Fig. 7.1. The tem-

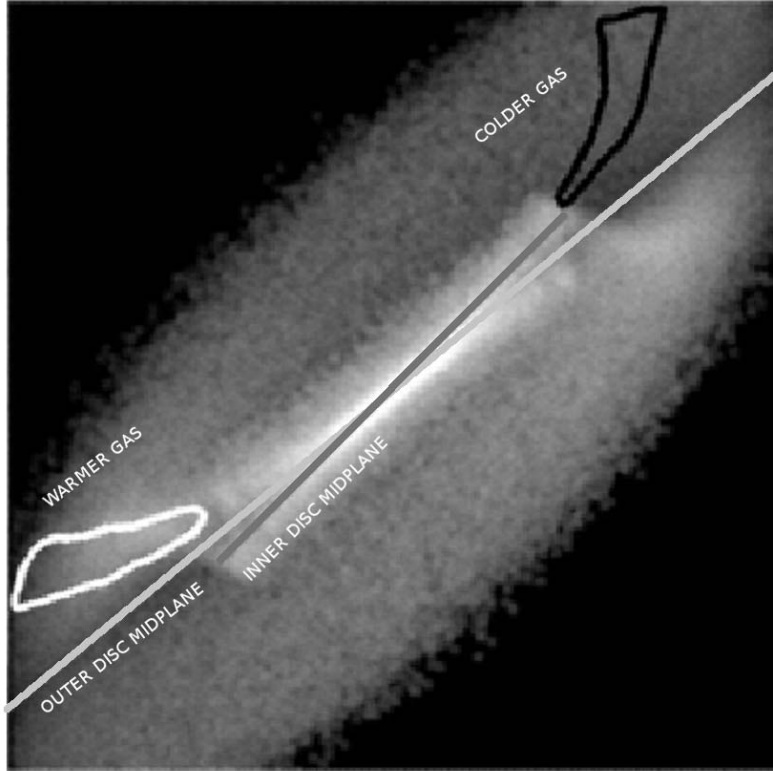


Figure 7.2: Illustration of a warped disc structure, in an edge-on projection. Straight light and dark grey lines show the plane of the disc and of the inner warped disc component, respectively. The white curve shows the surface region with a higher temperature, heated well by the star, and the black curve shows the cooler region partly obscured by the warp. The image of the disc with a 400 AU radius is adapted from Quillen (2006), where a detailed warped disc model is presented.

peratures of 40–60 K compare well to the theoretical predictions of the temperature in the regions where these lines saturate in discs (see Fig. 6 in van Zadelhoff et al. 2001). The difference in temperature between the two sides of the disc may be explained by a warped inner disc, as illustrated in Fig. 7.2, with the elevated side of the inner disc intercepting a fraction of stellar light that would otherwise reach the outer disc, while the opposite side is slightly more illuminated, with the inner part of the disc shifted downwards. The possibility of an inner warp is suggested by Quillen (2006) for HD 100546, with an inner component extending up to 200 AU inclined by $\approx 15^\circ$ with respect to the outer component extending beyond that radius.

The temperature asymmetry is possible also if the disc has a different thickness at the two sides. This may happen in a disc with dust settling underway, or if a planet or another body embedded in the disc stirs up the dust. In this case the ‘stirred up’ part of the disc intercepts more stellar light and becomes somewhat warmer. A companion body in HD 100546 is suggested in the literature, to explain the observed inner hole, gas kinematics, and spiral arms (Bouwman et al. 2003; Acke & van den Ancker 2006; Quillen et al. 2005).

Asymmetry in the disc spatial distribution. If one side of the disc extends slightly further out than the other (e.g., on the SE side), the increase in disc surface at that side will contribute to the line flux at one side of the spectral line causing line asymmetry. This may be a plausible explanation for the 3–2 line, but not the observed 6–5 line with a $9''$ beam size, unless the asymmetry is within 450 AU. Such an asymmetry may affect

the scattered light images of HD 100546, with the disc extending further to the SW than to the NE of the star. However this is not seen in the observations of Augereau et al. (2001). Furthermore, the additional emission from this region would dominate the frequencies closer to the line centre, and not the redshifted peak.

Disc density asymmetry. A different density on the two sides of the disc, with one side significantly denser than the other, may cause asymmetry in the molecular line emission. This scenario only applies if the observed line emission is at least marginally optically thin and thus sensitive to the disc midplane density. This seems unlikely, given the ratio between ^{12}CO and ^{13}CO $J=3-2$ lines, unless the isotopic fractionation is pronounced in this disc. If we decrease the disc mass to allow the ^{12}CO line emission in our models to be sensitive to the density variations in the midplane, we would have to assume a lower temperature in the calculations, close to the temperature in the disc midplane (10–30 K in the outer disc). While the asymmetry in the line profile can be reproduced in this way, the resulting lines would be much weaker than observed.

Pointing offset. A systematic pointing offset of APEX towards the SE of $\delta\text{RA}=1''.1$ and $\delta\text{Dec}=-1''.6$, well within the measured pointing accuracy of $3''$, may cause a line asymmetry as observed in the ^{12}CO $J=3-2$ and $J=6-5$ lines. Figure 7.3 shows the comparison between the observed spectra of the two lines and the spectra extracted from axially symmetric models using the abovementioned offset. The T_{100} parameter in these models is 50 K for the ^{12}CO $J=3-2$ and 60 K for the $J=6-5$ line. To explain the observations, the $1''.9$ pointing offset would need to be present in both our 2005 and 2008 data, thus consistent over a three year period. Given that the pointing model of the APEX telescope has been significantly improved over the period between the two observations, a consistent, systematic pointing error is unlikely. The stellar coordinates are also known to better than the required offset. Finally, in our APEX jiggle map obtained on 2008 November 10, the asymmetric profile corresponds to the pixel with the largest integrated intensity. We therefore conclude that a pointing offset is an unlikely explanation for the observed asymmetry, but cannot entirely rule out the possibility. Only future interferometric observations of this source can answer whether the apparent asymmetry is real or due to a pointing offset.

^{13}CO $J=3-2$ and ^{12}CO $J=7-6$ line fit

The ^{13}CO $J=3-2$ spectrum is suggestive of asymmetry, but the difference between the line intensity at the expected location of the two peaks is within the noise level. This line arises from denser and colder disc layers, distinct to those traced by the high- J transitions. A temperature asymmetry in the upper layers is unlikely to have a detectable effect on the temperature deeper in the disc, and it is likely that any future, high-sensitivity observations of optically thin CO isotopologue emission, C^{18}O for example, will reveal symmetric line profiles.

As in the calculations of Sect. 7.3.2, we use the RATRAN code, including Keplerian rotation and a disc inclination as above. No freeze-out is included. We adopt a constant ^{13}CO abundance, assuming an isotopic ratio $[^{12}\text{C}]/[^{13}\text{C}]=77$ (Wilson & Rood 1994). We fit the ^{13}CO $J=3-2$ spectrum assuming an axially symmetric temperature structure, with $T_{100}=25$ K. The comparison of the synthetic spectrum from our best-fit model to

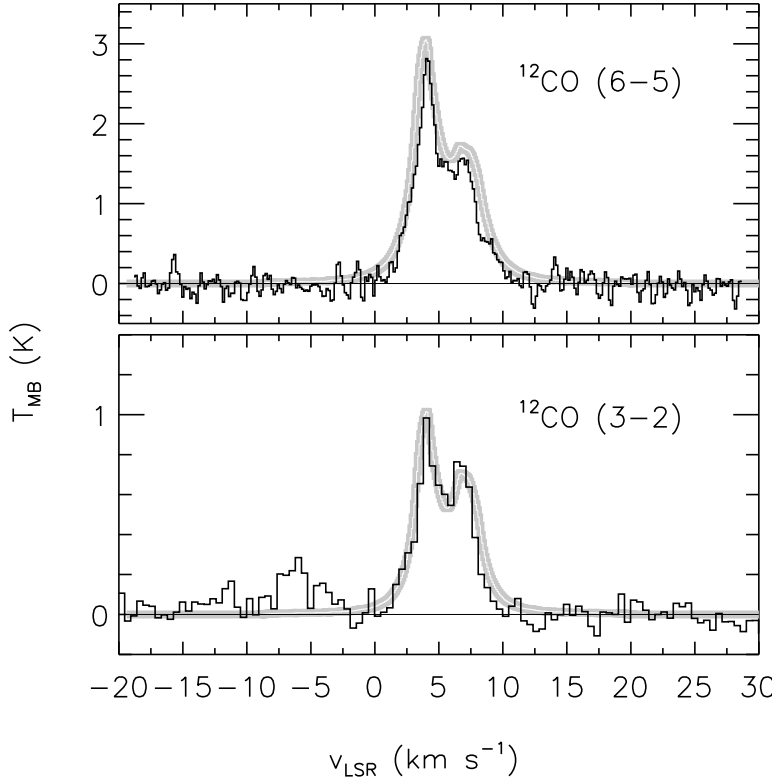


Figure 7.3: Spectra of the ^{12}CO $J=3-2$ and $J=6-5$ lines observed towards HD 100546, compared to the spectra from symmetric models with a pointing offset of $\delta\text{RA}=1''.1$ and $\delta\text{Dec}=-1''.6$.

the observations is shown in Fig. 7.1.

The ^{12}CO $J=7-6$ is fit with $T_{100}=50$ K, close to the temperatures used to fit the $J=6-5$ lines. These two transitions are energetically close and our data are consistent with the expectation that they should trace the same disc layers. The ^{12}CO $J=7-6$ line profile is therefore likely asymmetric, but this asymmetry is hidden in the noise of our observations.

7.3.3 ^{12}CO line ratios

As discussed in Sect. 7.2, the observed CO 6-5/3-2 integrated intensity ratio is 1.0 ± 0.2 when the observations are scaled to the same beam. This is a factor 2 higher than the ratios close to 0.5 found for the discs around the T Tauri stars LkCa 15 and TW Hya by van Zadelhoff et al. (2001) and Qi et al. (2006). The TW Hya 6-5/3-2 ratio has been interpreted as proof that the gas temperature is higher than that of the dust in the surface layers where gas and dust are not thermally coupled. Both UV radiation and X-rays have been invoked to provide the additional gas heating (Jonkheid et al. 2004; Kamp & Dullemond 2004; Glassgold et al. 2004; Nomura & Millar 2005; Gorti & Hollenbach 2008).

The higher ratio found for HD 100546 implies higher gas temperatures than for the T Tauri disks. This is expected based on models where most of the gas heating comes from UV radiation from the central star, since the cooler stars have less UV

radiation (e.g. Woitke et al. 2009). The gas temperature is also strongly affected by the PAH abundance in the disc. PAH features are seen prominently in the HD 100546 mid-infrared spectrum (e.g. Malfait et al. 1998), and have been shown to be spatially extended across the disk (Geers et al. 2007). In contrast, neither of the two T Tauri disks show PAH emission, implying typical PAH abundances a factor of 10–100 lower (Geers et al. 2006).

For the specific case of Herbig Ae disks, Jonkheid et al. (2007) have computed the gas heating and chemistry as well as the resulting CO 6–5 and 3–2 line emission starting from a set of dust disk models developed by Dullemond & Dominik (2005). Models with decreasing disk mass from 10^{-1} to $10^{-4} M_{\odot}$ and decreasing dust/gas ratios from 10^{-2} to 10^{-6} (simulating grain growth and settling) were investigated. For Herbig stars, X-rays can be neglected (Kamp et al. 2008), so all the heating is through UV radiation. The UV radiation field was taken to be that of a B9.5 star, very close to that expected for HD 100546. An accurate treatment of the shape of the UV field at short wavelengths, $<1100 \text{ \AA}$, is very important for a correct calculation of the CO photodissociation and atomic carbon photoionization rates, since the UV intensity of a B9 star is orders of magnitude weaker in this wavelength range than the (scaled) standard interstellar radiation field. The PAH abundance is taken to follow the dust/gas ratio, with an abundance of 10^{-7} for a normal dust/gas ratio=100.

The resulting ^{12}CO $J=6-5/3-2$ integrated intensity ratios computed by Jonkheid et al. (2007) summed over the full extent of the disk model are remarkably close to unity for the entire range of disk parameters investigated. The absolute ^{12}CO and ^{13}CO intensities for model B2 (a disk with a mass of $0.01 M_{\odot}$ with a standard gas/dust ratio of 100, appropriate for HD 100546) are also within 40% of the observed values when scaled to the same source distance and beam size, indicating a good agreement between models and observations.

7.3.4 Implications of the [C I] $J=2-1$ non-detection

Figure 1 includes the high-quality spectrum around the [C I] $J=2-1$ line at 809.344 GHz. No significant feature is detected down to 0.3 K rms in a 0.27 km s^{-1} velocity bin, implying a limit on the integrated intensity of $\approx 1.5 \text{ K km s}^{-1}$ over the range 0–10 km s^{-1} (same width as for the detected ^{12}CO lines). Model B2 of Jonkheid et al. (2007) predicts integrated [C I] intensities, scaled to the distance of HD 100546, around 15–20 K km s^{-1} , whereas the model intensities are even larger in disks with significant grain growth and settling (BL model series). Thus, while the CO data appear entirely consistent with their sophisticated UV-heated disk atmosphere models, the [C I] data are clearly discrepant by an order of magnitude.

One possible solution could be that the radiation field contains more carbon ionizing photons than assumed here, shifting the chemical balance from neutral to ionized atomic carbon. Indeed, the predicted [C II] line intensities for the model disks of Jonkheid et al. (2007) are very low, $<0.1 \text{ K km s}^{-1}$, whereas they are more than an order of magnitude higher for disks around T Tauri stars with excess UV emission (Jonkheid et al. 2004). Such excess of UV emission could come from the disk-star accretion bound-

ary layer. Indeed, HD 100546 is observed to undergo significant accretion, in spite of the known (dust) gap in the inner disk (Vieira et al. 1999). Searches for the [C II] line with the HIFI instrument on the Herschel Space Observatory can test this scenario. In this case, the [C I] line intensity and the [C II]/[C I] line ratio could be a diagnostic of the presence of excess UV emission over that of the stellar photosphere.

7.3.5 Implications for the dust continuum emission

Our assumed gas mass of $0.01 M_{\odot}$ corresponds to $10^{-4} M_{\odot}$ of dust adopting a gas-to-dust mass ratio of 100. To calculate continuum fluxes, we assume that the dust emission is optically thin and arises at temperatures close to 25 K, the 100 AU temperature found to fit the ^{13}CO line emission well. With these parameters, the dust continuum flux at 3.4 mm of 36 mJy reported in the observations of Wilner et al. (2003) at $2''$ resolution and the flux at 1.3 mm of 690 mJy reported by Henning et al. (1998) at $23''$ resolution can both be fitted with a dust emissivity $\kappa_{1.3\text{ mm}} = 0.1 \times (1.3\text{ mm}/\lambda\text{ (mm)})^{0.9}$, representative of grain growth to sizes of 100 cm in discs (Draine 2006). A shallow slope of the emissivity of $\beta \approx 1.0$ is also suggested by Wilner et al. (2003).

7.4 CONCLUSIONS

We summarise our conclusions as follows:

- We present evidence for abundant warm molecular gas associated with the disc around HD 100546, in regions within ~ 400 AU from the star, successfully separated from more extended material in our CHAMP⁺ observations;
- The gas kinematics are consistent with Keplerian rotation around an $2.5 M_{\odot}$ star of a disc with a 400 AU radius, viewed at an inclination of 50° from face-on;
- The ^{12}CO (6–5)/(3–2) line ratio of 1.0 ± 0.2 is a factor of two higher than measured towards discs around T Tauri stars, likely due to a stronger UV radiation from the star;
- Line asymmetry seen in the ^{12}CO $J=6-5$ and $J=3-2$ lines can be explained by a temperature asymmetry, with one side of the disc slightly colder than the other, possibly due to a partial obscuration of one side by a warped inner disc or a high disc rim, but a systematic pointing offset of the telescope is also possible;
- Our data are consistent with a total disc mass of $0.01 M_{\odot}$. We exclude the possibility of a low-density disc and optically thin ^{12}CO emission, as the disc midplane temperature is insufficient to reproduce the observed line intensities. Furthermore, efficient freeze out at low temperatures would limit the emission to a much smaller radius, altering the line profile.
- The puzzling non-detection of [C I] $J=2-1$ line may indicate efficient photoionisation.

Future observations with ALMA will be crucial to characterise the disc around HD 100546, spatially resolve its kinematics and structure. In particular, such observations will allow a detailed comparison between the spatial distribution of the gas traced by rotational transitions of ^{12}CO and its isotopologues, and the dust traced by millimetre continuum emission.

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