CO ro-vibrational lines in HD 100546
A search for disc asymmetries and the role of fluorescence**

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ABSTRACT

Aims. We have studied the emission of CO ro-vibrational lines in the disc around the Herbig Be star HD 100546 to determine physical properties, disc asymmetries, the CO excitation mechanism, and the spatial extent of the emission, with the final goal of using the CO ro-vibrational lines as a diagnostic to understand inner disc structure in the context of planet formation.

Methods. High-spectral-resolution infrared spectra of CO ro-vibrational emission at eight different position angles were taken with the CRyogenic high-resolution InfraRed Echelle Spectrograph (CRIRES) at the Very Large Telescope (VLT). From these spectra flux tables, line profiles for individual CO ro-vibrational transitions, co-added line profiles, and population diagrams were produced. We have investigated variations in the line profile shapes and line strengths as a function of slit position angle. We used the thermochemical disc modelling code ProDiMo based on the chemistry, radiation field, and temperature structure of a previously published model for HD 100546. We calculated line fluxes and profiles for the whole set of observed CO ro-vibrational transitions using a large CO model molecule that includes the lowest two electronic states, each with 7 vibrational levels and within them 60 rotational levels.

Results. The observed CO ro-vibrational lines are largely emitted from the inner rim of the outer disc at 10–13 AU. The line shapes are similar for all v levels and line fluxes from all vibrational levels vary only within one order of magnitude. All line profile asymmetries and variations can be explained with a symmetric disc model to which a slit correction and pointing offset is applied. Because the angular size of the CO emitting region (10–13 AU) and the slit width are comparable the line profiles are very sensitive to the placing of the slit. The model reproduces the line shapes and the fluxes of the v = 1–0 lines as well as the spatial extent of the CO ro-vibrational emission. It does not reproduce the observed band ratios of 0.5–0.2 with higher vibrational bands. We find that lower gas volume densities at the surface of the inner rim of the outer disc can make the fluorescence pumping more efficient and reproduce the observed band ratios.

Key words. protoplanetary disks – line: profiles – stars: individual: HD 100546 – stars: variables: T Tauri – circumstellar matter – stars: variables: Herbig Ae/Be

1. Introduction

The inner regions of protoplanetary discs are excellent laboratories for studying the formation of planets. At high spectral resolution, line profiles of various gas species contain a wealth of physical, chemical, and kinematic information. The CO ro-vibrational lines around 4.7 μm have been shown to originate in the innermost regions of the discs (Najita et al. 2000; Brittain et al. 2003; Blake & Boogert 2004). Holes or gaps due to planet formation can be directly traced in the line profiles of these CO ro-vibrational transitions (Regály et al. 2010). If CO is to be used as a probe, it is crucial that we understand the CO ro-vibrational lines in terms of the chemistry and line radiative transfer. We need to understand what governs line strengths and shapes and where the emission originates.

Comparing modelled and observed data, Brittain et al. (2007) found that UV fluorescence can be an important excitation mechanism for the CO in dust-depleted discs. From the implementation of a large CO model molecule in the
radiative thermo-chemical protoplanetary disc code ProDiMo, Thi et al. (2013) confirmed that UV fluorescence has a significant impact on the population of the ro-vibrational levels of the CO molecule. The main effect of the UV pumping is populating the $v > 1$ levels.

A particularly well known Herbig Be star is HD 100546, spectral type B9Vne, with a protoplanetary disc. It has been observed and analysed by several authors. In coronagraphic imaging, HD 100546 has shown a large-scale envelope and a disc that extends out to 515 AU with an asymmetric brightness profile (Grady et al. 2001). From its position in the Hertzsprung-Russell diagram the age of the star has been estimated to about 10 Myr (van den Ancker et al. 1997). The infrared spectrum of HD 100546 shows exceptionally strong emission from crystalline silicates, suggesting a highly processed grain population, probably associated with the inner rim region of the outer disc (Malfait et al. 1998). The disc has been classified as transitional with a gap from 4–13 AU (Grady et al. 2005) and a disc wall at 10–13 AU (from here on referred to as the disc wall). The gap might be caused by the presence of a giant planet or substellar companion (Acke & van den Ancker 2006). Located at a distance of 103 pc (van den Ancker et al. 1998), the disc is spatially resolved on scales of $0.1$ corresponding to 10 AU. The disc inclination has been constrained to $i = 42 \pm 5$ and the position angle (PA) to $PA = 145 \pm 5$ (Ardila et al. 2007). The presence of molecular gas in the outer disc has been confirmed, with observations of CO pure rotational lines (Panić et al. 2010). Based on these observations and new data from the Herschel Space Observatory, Bruderer et al. (2012) modelled the disc and concluded that the highest CO rotational lines are emitted from ~20–50 AU, the mid J lines from ~40–90 AU, and the low J lines trace the outer disc. Furthermore, they favour a disc model with a gas/dust ratio of 100 with only a small fraction of volatile carbon. Benisty et al. (2010) presented observations from the VLTI Interferometer using the AMBER instrument and obtained 26 visibilities in the [2.06–2.46] $\mu$m wavelength range and derived basic characteristics of the NIR emission. Their visibility curve is almost flat with wavelength, while the uniform brightness ring predicts a slightly steeper slope. The interferometric observations are consistent with a disc model that includes a gap until ~13 AU from the star and a total dust mass of ~0.008 lunar mass inside it. Tatulli et al. (2011) aimed to refine the disc model presented in Benisty et al. (2010). Using interferometric data from the AMBER/VLTI instrument in the H- and K-band, they spatially resolved the warm inner disc and constrained the structure. Combining these with photometric observations they analysed the data using a passive disc model based on three dimensional Monte-Carlo radiative transfer. They found that the spectral energy distribution (SED) from the UV to mm range and the near-infrared (NIR) data was adequately reproduced by their model composed of a tenuous inner disc (0.24–4 AU) with a dust mass of ~1.75 $\times 10^{-10}$ $M_\odot$, a gap devoid of dust and a massive outer disc (13–500 AU) with a dust mass of ~4.3 $\times 10^{-8}$ $M_\odot$. Recent dust observations have revealed an inner disc that extends to no farther than 0.7 AU from the star with a following gap of about 10 AU (Panić et al. 2014). Furthermore, the authors found this inner disc to be asymmetric, while the disc wall at 10 AU is fully symmetric.

The CO ro-vibrational transition lines at 4.7 $\mu$m emitted from HD 100546, have been observed and studied and a lack of CO emission from small radii (<10 AU) has been documented (van der Plas et al. 2009; Brittain et al. 2009). It has been shown that the lack of CO cannot be caused by a completely gas-free inner disc, since [OI] 6300 Å emission has been observed from the disc (Acke & van den Ancker 2006). The main formation mechanism of [OI] 6300 Å emission is thought to be dissociation of OH. A detection of [OI] 6300 Å emission thereby suggests the presence of molecular gas in the inner disc. However, Liskowsky et al. (2012) presented an OH spectrum from the disc and do not detect OH from small radii. Thermo-chemical modelling of the CH$^+$ emission observed with the Herschel Space Observatory in HD 100546 suggests that CH$^+$ is mostly located at the second ring (10–13 AU) (Thi et al. 2011). The same could be the case for CO, since no emission has been observed at smaller radii. Goto et al. (2012) resolved the CO vibrational line emission from HD 100546 with $0'1$ angular resolution using the CRIRES instrument and found unambiguous evidence of a warm disc atmosphere far away from the central star including a CO emitting region extending out to as far as 50 AU. Recently Liskowsky et al. (2012) and Brittain et al. (2013) confirm the lack of CO emission from small radii. With a $0'34$ slit and a spatial resolution of $0'4$–$0'8$, they find the main part of the CO emission to be consistent with an axisymmetric disc. Meanwhile gathering observations spanning several years, a periodically occurring asymmetry was detected only in the $v = 1$–0 lines (Brittain et al. 2013).

In this paper we compare a detailed model with observational data using the CRIRES observations of the CO ro-vibrational emission from HD 100546 from Goto et al. (2012) and the corresponding modelled emission predicted by the thermo-chemical protoplanetary disc model ProDiMo (Woitke et al. 2009). This includes the comparison of line shapes, line strengths, and line ratios. The possibility of disc asymmetries is investigated. The goal is to test our understanding of the complex coupling between chemistry, IR and UV fluorescence, and radiative transfer, to assess the potential of the CO ro-vibrational emission lines as probes for the inner disc geometry.

First we present our CRIRES observations of HD 100546 (Sect. 2) and describe our data reduction method (Sect. 3). We then produce average line profiles and derive population diagrams (Sect. 4). In Sect. 5, we present the ProDiMo model of HD 100546 with a large CO model molecule combined with a slit simulator. We explore the variety of line shapes that could come from changes in slit position and we produce modelled line profiles and population diagrams to be compared to the observational data. We finish the paper by comparing the observed results with the modelled results (Sects. 5 and 6) and discuss possible solutions to some remaining inconsistencies between model and observations. We present our observational slit analysis and our modelled slit effects in the appendix.

2. Observations

High resolution spectra of HD 100546 ($\Delta v = 3$ km s$^{-1}$, $R = 100000$) were obtained on 29 and 30 March 2010 UT with the VLT CRYogenic high-resolution InfraRed Echelle Spectrograph (CRIRES; Goto et al. 2012). The wavelength interval between 4.6 to 5.0 $\mu$m was continuously covered with six different grating settings. The spectra were recorded by rotating the slit (slit width $= 0'2$) to PA = 145°, 55°, 10°, 100° and their respective anti-parallel positions to increase the spatial coverage (see Fig. 1 for a view of the slit coverage). The telescope was nodded by 10° along the slit after each second exposure to subtrac the sky emission and the dark current. The bright telluric standard stars, HR 6556 (A5III) and HR 6879 (B9.5II), were observed to remove the telluric absorption lines. The spectroscopic flat fields were collected in the morning after the observations.
with the same instrumental settings as used for the science observations. Table 1 provides a summary of the observations and Fig. 1 shows a schematic drawing of how the slit is positioned with respect to the disc wall at the various PA.

In our dataset, we found clear variations in the shape of line profiles observed at different position angles. These variations are caused by a varying slit loss. The details of this are discussed in Appendix A.

### 3. Data reduction and analysis

#### 3.1. Spectroscopy

The science data was reduced using the CRIRES pipeline recipes ver. 1.11.0 on esorex platform ver. 3.8.1 and was corrected for the detector non-linearity and response. The observations where done in nodding mode: The spectra are nodded between two positions (A and B) $10''$ apart on the sky in the pattern ABBA so that the source is in different positions on the chip. The sky emission was removed by subtracting the nodded A and B spectra. The spectrograms were registered and combined, and one dimensional spectra were extracted for each grating setting and slit position angle. The rectangular extraction method was used. The width of the extracted rectangle was 41 pixels $= 3''.53$. The data of the spectroscopic standard stars (HR 6556 and HR 6879) were reduced in the same way. The spectra of HD 100546 were divided by those of the standard stars after making small adjustments in the optical depth of the telluric lines, the wavelength, and the spectral resolution. These adjustments are done to remove the telluric lines as clean as possible. The wavelength calibration was performed by matching the telluric lines to the model atmospheric transmission spectra calculated using the LBLRTM code (Clough et al. 2005). The calibration accuracy is better than $1 \text{ km s}^{-1}$.

#### 3.2. Flux calibration

There are several records of $M$-band photometry published. In 1988 the $M$-band magnitude was measured to $m_M = 3.75 \pm 0.06$ (de Winter et al. 2001), where $m_M$ refers to the apparent magnitude. In 1991, the ESO 1 m Schmidt telescope ($\lambda_{\text{mean}} = 4.6 \mu m$) measured $m_M = 3.76$ (Fouque et al. 1992); In 1992, Garcia-Lario et al. (1997) obtained $m_M = 3.79 \pm 0.07$. In 2009, HD 100546 was observed by the Wide-Field Infrared Survey Explorer (WISE), and the $W2$ brightness ($\lambda_{\text{mean}} = 4.6 \mu m$) was measured to $m_M = 3.156 \pm 0.049$. However for sources brighter than magnitude 6, the WISE band 2 fluxes suffer from saturation effects and are therefore unreliable (Padgett, priv. comm.).

For our analysis, we calibrate the continuum level of HD 100546 to the spectroscopic standards. The $M$-band photometry of the standard stars, HR 6556 ($m_M = 1.62$ mag) and HR 6879 ($m_M = 1.70$ mag), was observed at the ESO 1-m telescope with the standard ESO NIR filter set ($\lambda_c = 4.46 \mu m$, $\Delta \lambda = 0.8 \mu m$). The continuum flux of HD 100546 (for the spectra taken with PA = 145° at reference wavelength $\lambda = 4.782 \mu m$) after division by the STD was 9.73 Jy at the mean wavelength of the filter 4.750 $\mu m$. This is about a factor of 1.7 brighter than the above listed $M$-band photometry measurements. The error expected from the difference in the continuum slopes in HD 100546 and the standard star is 10–15%. If our flux calibration is correct, HD 100546 is getting brighter by ~70% over the baseline of 18 years. Herbig stars are known to be intrinsically variable, and even the disc luminosity of some Herbig Ae/Be stars is known to change on short timescales (Bibo & The 1991; Sitko et al. 1994; Eiroa et al. 2002). For HD 100546, in particular, NIR variability has been documented: in the $K$-band a 0.5 mag decrease over a span of seven years and in the $L$-band a 0.8 mag decrease over the span of 20 years (Brittain et al. 2013). Furthermore, Brittain et al. (2013) find the CO ro-vibrational hot band emission ($\Delta v = 1, v' > 1$) to brighten over a span of eight years, and suggest this could be due to a 0.4 mag variation in the $M$-band flux. Thus, changes in the $M$-band continuum are not unlikely, but a follow up observation

### Table 1. Observational settings and conditions.

| Date  | $\lambda_{\text{eff}}$ [\(\mu m\)] | PA     | it [min] | STD     |
|-------|----------------------------------|--------|---------|---------|
| 29/3  | 4662 145°/325°/55°/235°          | 1      | HR 6556 |
| 2010  | 4.676 145°/325°/55°/235°         | 1      | HR 6556 |
|       | 4.929 145°/325°/55°/235°         | 1      | HR 6556 |
|       | 4.957 145°/325°/55°/235°         | 1      | HR 6556 |
| PSF~  | 0.169°                            |        |         |         |

| Date  | $\lambda_{\text{eff}}$ [\(\mu m\)] | PA     | it [min] | STD     |
|-------|----------------------------------|--------|---------|---------|
| 30/3  | 4.662 10°/190°/100°/280°          | 1      | HR 6879 |
| 2010  | 4.676 10°/190°/100°/280°          | 1      | HR 6879 |
|       | 4.782 145°/325°/55°/235°         | 1      | HR 6879 |
|       | 4.796 145°/325°/55°/235°         | 1      | HR 6879 |
| PSF~  | 0.186°                            |        |         |         |

**Notes.** For each science spectra the associated telluric standard stars (STD) are listed. For each of the two observing nights the respective four wavelength settings are listed. For each wavelength setting four different position angles were taken. The PSF FWHM was measured at several locations in the STD spectra for each wavelength settings and the table lists an average, for each day.
measuring the $M$-band magnitude should be done in order to confirm this increase in luminosity.

Our data suffers from slit loss both for the continuum and the lines. If we calibrate to previous measurements of the continuum, we lose the natural variation in fluxes between spectra taken at different position angles. However, this is exactly what we aim to explore. We will therefore use the spectra calibrated to the spectroscopic standard for the analysis hereafter (Table 3).

### 3.3. Line detection and selection

For our full data set covering six different wavelength settings the quality of the data varies. For the 29th and the 30th respectively the Strehl ratio (the efficiency of the AO system) was $\sim 42\%$ and $\sim 28\%$ in the $K$-band. This corresponds to Strehl ratios at our wavelength settings of $\sim 80\%$ on the 29th and a few percentages lower on the 30th. For CRIRES a good correction in the $K$-band typically corresponds to a Strehl ratio higher than $30\%$ (CRIRES manual). The wavelength settings 4.662 $\mu$m and 4.676 $\mu$m observed on the 29th have the highest quality. The spectra from the wavelength settings 4.782 and 4.796 $\mu$m were so noisy that it was necessary to convolve the signal with a Gaussian kernel in order to detect more than just a few lines.

Within each spectrum the detected lines also vary in quality. Chip 1 and 4 are more noisy than chip 2 and 3. Some lines fall closer to telluric lines and residuals can be left in the STD filtered spectra. Finally many lines are blended and hard to separate. We thus manually select the best undistorted and unblended lines for further line profile analysis and comparison with models. For the two observing nights different wavelength regions are covered and the line samples from the two nights are thereby different. We detect lines all the way up to $\nu = 6$–$5$, but the higher $\nu$-bands have low S/N profiles and not enough lines for good statistics.

Figure 2 shows the full spectrum from the wavelength setting of 4.662 $\mu$m (chip 3) at a position angle of 145°.

### 4. Results

Table 2 presents a full listing of our selected unblended and clean CO ro-vibrational lines. For all these CO ro-vibrational transitions, line profiles (flux as a function of velocity) have been extracted. The individual line profiles are normalized by their fitted continuum, shifted to zero continuum and the line profile is then normalized to the maximum flux value. Lines from different ro-vibrational transitions show very similar shape. Thus, we can make average profiles collecting all the individual transitions. The profiles are combined to median profiles (one for each PA). The details of this are described in Appendix A and the profiles are shown in Fig. A.2. Integrating each line separately, individual line fluxes are derived. For PA = 145° these are listed in Table 3.

#### 4.1. Population diagrams

If (1) all CO comes from a region with a single temperature $T_{\text{rot}} = T_{\text{gas}}$, (2) the CO gas is in local thermodynamical equilibrium (LTE), and (3) the lines are optically thin, we can write the Boltzmann equation as:

$$ N_{i,j} = \frac{N_g}{Q_{\text{rot}}(T_{\text{rot}})} e^{\frac{-E_J}{kT}}. $$  \hspace{1cm} (1)

We can calculate the ratio $N_{i,j}/g_j$ from the observed line flux:

$$ \frac{N_{i,j}}{g_{i,j}} = \frac{4\pi F_{i,j}}{g_{i,j}h\nu_{i,j}A_{i,j} \cdot \Omega}. $$  \hspace{1cm} (2)

In the above equations $N_{i,j}$ is the column density of the upper level, $E_j$ its energy, $g_{i,j}$ its statistical weight, $Q_{\text{rot}}$ is the rotational
Table 2. CO ro-vibrational line sample.

| v  | \(\nu = 0\) | \(\nu = 1\) | \(\nu = 2\) | \(\nu = 3\) | \(\nu = 4\) |
|----|-------------|-------------|-------------|-------------|-------------|
| e-band | wl.set[\(\mu m\)] | Transition | wl.set[\(\mu m\)] | Transition | wl.set[\(\mu m\)] | Transition |
| 29/3 | | | | | |
| v = 1–0 | 4.929 | P21, P26, P27, P30 | 4.957 | P26, P22 | |
| v = 2–1 | 4.662 | R4, R6, R8 R10, R11, R12, R14 | 4.676 | R4, R5, R6, R8, R9, R10, R12, R13, R14 | 4.929 | P21, P25 |
| v = 3–2 | 4.662 | R14, R17, R18, R20, R23 | 4.929 | P23, P27 | 4.957 | P23, P27 | |
| v = 4–3 | 4.662 | R14, R17, R18, R20, R23 | 4.929 | P23, R27 | 4.676 | R14, R17, R18, R20, R23 | |
| 30/3 | | | | | |
| v = 1–0 | 4.782 | P12, P13, P14, P17 | 4.796 | P8, P11, P12, P14, P17 | |
| v = 2–1 | 4.662 | R4, R6, R8, R10, R11, R12, R14, R16 | 4.676 | R4, R5, R6, R8, R9, R10, R13, R14 | 4.782 | P7 |
| v = 3–2 | 4.662 | R14, R17, R18, R20, R23 | 4.782 | P1, R5 | 4.796 | P8, P11 |
| v = 4–3 | 4.662 | R23, R27, R29 | 4.782 | P10, R11, R13 | 4.796 | R8, R12, R13 |

Notes. These are the lines used throughout the paper. Shown are only lines not contaminated by blends or telluric lines.

Table 3. Line fluxes from data collected on the 29th at PA = 145°.

| Line ID | \(\lambda_{\text{line}}\) [\(\mu m\)] | \(F_{\text{Total}}\) \(10^{-15} \text{ erg cm}^{-2} \text{s}^{-1}\) | Error |
|--------|------------------|-------------------|-------|
| \(1–0)P21 | 4.8622 | 55.7 | 0.7 |
| \(1–0)P22 | 4.8760 | 67.8 | 0.7 |
| \(1–0)P26 | 4.9204 | 42.7 | 1.1 |
| \(1–0)P27 | 4.9204 | 57.5 | 1.2 |
| \(1–0)P30 | 4.9668 | 61.4 | 1.4 |
| \(1–0)P27 | 4.9318 | 42.3 | 1.1 |
| \(1–2)P25 | 4.9716 | 22.3 | 0.9 |
| \(1–2)P21 | 4.9269 | 26.9 | 1.0 |
| \(1–2)P23 | 4.9490 | 24.6 | 0.5 |
| \(1–2)P27 | 4.9947 | 33.3 | 1.7 |
| \(1–2)R04 | 4.6831 | 30.5 | 1.6 |
| \(1–2)R06 | 4.6675 | 42.9 | 1.6 |
| \(1–2)R08 | 4.6523 | 37.4 | 1.3 |
| \(1–2)R09 | 4.6484 | 42.9 | 0.7 |
| \(1–2)R10 | 4.6374 | 37.1 | 0.5 |
| \(1–2)R10 | 4.6374 | 29.4 | 0.5 |
| \(1–2)R11 | 4.6301 | 28.4 | 1.1 |
| \(1–2)R12 | 4.6230 | 35.9 | 5.2 |
| \(1–2)R12 | 4.6230 | 46.1 | 1.7 |
| \(1–2)R13 | 4.6160 | 33.3 | 0.6 |
| \(1–2)R14 | 4.6090 | 24.3 | 1.0 |
| \(1–2)R14 | 4.6090 | 37.2 | 0.8 |
| \(1–2)R08 | 4.6523 | 39.9 | 1.8 |
| \(1–2)R04 | 4.6831 | 23.8 | 1.1 |
| \(1–2)R05 | 4.6752 | 31.7 | 1.2 |
| \(1–2)R06 | 4.6675 | 38.8 | 1.1 |
| \(2–1)P21 | 4.9901 | 21.1 | 1.3 |
| \(2–1)P15 | 4.9257 | 19.3 | 0.8 |
| \(2–1)P15 | 4.9257 | 30.2 | 1.0 |
| \(2–1)P14 | 4.9154 | 15.4 | 0.8 |
| \(2–1)P14 | 4.9154 | 16.3 | 0.5 |
| \(2–1)P11 | 4.8853 | 15.7 | 1.2 |
| \(2–1)P07 | 4.8468 | 15.3 | 1.1 |
| \(2–1)R14 | 4.6670 | 25.9 | 1.0 |
| \(2–1)R17 | 4.6464 | 21.1 | 0.5 |
| \(2–1)R18 | 4.6398 | 26.8 | 0.7 |
| \(2–1)R20 | 4.6268 | 21.0 | 0.3 |
| \(2–1)R20 | 4.6268 | 20.9 | 0.3 |
| \(2–1)R23 | 4.6080 | 21.8 | 0.8 |
| \(2–1)R23 | 4.6080 | 18.6 | 0.4 |
| \(4–3)P08 | 4.9185 | 12.9 | 1.0 |
| \(4–3)R29 | 4.6311 | 15.3 | 0.9 |
| \(4–3)R27 | 4.6425 | 20.9 | 0.5 |
| \(4–3)R27 | 4.6425 | 17.0 | 0.4 |
| \(4–3)R23 | 4.6665 | 14.4 | 0.7 |

Notes. The flux error is found from the standard deviation (1σ) of the nearby continuum. The lines that occur twice are collected from different wavelength settings. The wavelengths of the individual lines are taken from Chandra et al. (1996).

For the vibrational temperature of the CO gas, we obtain the following equation:

\[
N_g = \sum_J N_J g_J \frac{N_{CO}}{Q_{vib}(T_{vib})} e^{-\epsilon_{vib} \theta_{vib}}. \tag{4}
\]

Thus, summing over \(N_g g_J\) from Eq. (2), for each \(v\)-band separately, we can construct a vibrational diagram of \(\ln(\sum_j N_g g_J)\) versus the ground level energy for each \(v\) level. We can then find the vibrational temperature \(T_{vib}\) using the same approach as above for the rotational temperature. It is important to state that we are not complete in \(J\) levels and therefore our \(T_{vib}\) determination is
points. The vibrational diagram from the two sets of simulated lines so the corresponding line has only been fitted from three points. The vibrational diagram from the two sets of simulated lines (different slit filter settings) from the model are also included in the plot (derived and discussed in Sect. 5.4).

We derive vibrational temperatures from our 29th line sample of \( T_{\text{vib}} = 2968 \, \text{K} \) and \( T_{\text{vib}} = 2978 \, \text{K} \) respectively for the PA settings 55° and 145° and for the 30th line sample of \( T_{\text{vib}} = 2040 \, \text{K} \) and \( T_{\text{vib}} = 2081 \, \text{K} \) respectively for the PA settings 10° and 100°. There is no significant difference in vibrational temperatures derived from the same date with orthogonal PA settings. The difference between the vibrational temperatures derived on the two separate nights comes from the lack of \( v = 1–0 \) lines detected at the PA settings of 10° and 100°. If we were to exclude the \( v = 1–0 \) lines from the vibrational temperature fit done for the 29th, we would find values similar to those derived from the 30th.

Observations generally cover a small subset of all \( J \) levels within each \( v \)-band. This can have a strong impact on the slope of the fit in the vibrational diagram. Some authors use the partition function to estimate the full population of each \( v \)-band from the slope and y-intersection of the rotational diagram. In this way the population is not affected by the amount of lines detected at each \( v \)-band. Meanwhile, a sampling bias can still be present due to the range of \( J \) levels used in the rotational diagram (strong curvature present at low \( J \) levels). In our sample, many detectable \( v = 1–0 \) lines were discarded because of strong telluric absorption. Furthermore, we did not detect lines beyond \( J = 30 \) and only a few lines of the \( v = 5–4, v = 6–5 \) bands (not included in the vibrational diagram). This has affected our derivation of vibrational temperatures. Since other papers use very different samples of lines and even numbers of lines, a direct comparison between vibrational temperatures become difficult.

For the modelling of CO ro-vibrational lines in this paper, we use the above described ProDiMo model for HD 100546, with the complete CO ro-vibrational molecular model, described in Thi et al. (2013). The collisional rate coefficients are gathered from the literature and scaled to extrapolate missing ones and the CO ro-vibrational transition probabilities are from Chandra et al. (1996). We include fluorescence pumping to the \( A^{1} \) electronic level and 60 rotational levels within 7 vibrational levels of both

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**Fig. 3.** Vibrational diagram for all transitions observed on the 29th at PA = 55°/145° and on the 30th at PA = 10°/100° (the individual lines are listed in Table 2). The error bars are smaller than the plotting symbols. For PA = 10°/100° the line sample does not include any \( v = 1–0 \), transitions so the corresponding line has only been fitted from three points.
Table 4. Key parameters used in our modelling of HD 100546.

| Parameter          | Value       |
|--------------------|-------------|
| Stellar mass       | $M_* = 2.4 M_\odot$ |
| Star radius        | $R_* = 1.54 R_\odot$ |
| Stellar luminosity | $L_* = 26 L_\odot$ |
| Gravity log (g)    | 4.36        |
| Gas mass           | $M_{\text{gas}} = 3.82 \times 10^{-4} M_\odot$ |
| Inner radius       | $R_{\text{in}} = 0.19$ AU |
| Outer radius       | $R_{\text{out}} = 500$ AU |

Notes. The parameters not shown here are the same as in Thi et al. (2011).

The ground electronic state $X^1\Sigma^+$ and the excited state $A^1\Pi$. We model the full set of observed lines listed in Table 2.

The gas density profile, the stellar UV field strength, the CO abundance, the gas temperature and the CO ro-vibrational band intensities are calculated in the Monte Carlo method. The cumulative line fluxes of the three representative lines, $v$-(1–0)R20, $v$-(2–1)R20, and (3–2)R20 are shown in Fig. 5. Our model indicates that most of the CO ro-vibrational line emission builds up in a narrow region at the disc wall (10–13 AU). At radii <10 AU the CO abundance is too low and beyond 15 AU the fluorescence mechanism becomes less efficient. The gas temperature contour plot shows that the temperature reaches 1000–5000 K in the region around 10–13 AU at heights 1–10 AU. If we look at the cumulative flux plot (Fig. 5) we see that about 50% of the line flux is coming from this small region, while the total line flux builds up out to ~20 AU (in the case of low $J$ lines up to 30–40 AU). The spatial extent of the observed CO emission drops to 1/10th of the maximum value at about ~40 AU (Goto et al. 2012). The modelled CO emission is less extended (see Fig. 5), but convolution with a Gaussian beam of 0′′17 gives a spatial extent (1/10th of maximum) of 28 AU. We expect an uncertainty for the spatial extent of <12 AU (the size of PSF). However, it is important to note that the observed spatial profile is calculated for a range of observed $\nu = 2$–1 lines, while our modelled spatial profile is calculated from one line ($v$-(2–1)R06). The model predictions for the $\Delta \nu = 2$, CO overtone emission at 2.3 $\mu$m show lines around $\sim 2 \times 10^{-16}$ erg/cm$^2$/s, consistent with the non detection of these lines (three sigma upper limit: $\sim 8.08 \times 10^{-15}$ erg/cm$^2$/s, van der Plas et al., in prep.).

5.3. Modelled line profiles

ProDiMo outputs line data cubes for each chosen CO ro-vibrational transition. Each cube contains a 201 $\times$ 201 pixel coordinate grid in units of AU and the spectral intensity in [erg/cm$^2$/s/Hz/sr] at every spatial position in the described coordinate grid for each of the 91 velocity channels, covering $\pm 20$ km s$^{-1}$ to $\pm 20$ km s$^{-1}$ and the continuum (see Appendix B). From this cube we create line images, profiles, and flux tables. They are our modelled “observations”. Each cube is piped through a slit filtering IDL procedure to add observational effects (Appendix A.2.1).

The final modelled line profiles, with the observations overplotted, are shown in Fig. 6. Here, a slit pointing offset of 0′′06 is imposed (the choice of offset is discussed in Appendix A.2.1). The upper two frames show that the line shape variations from

1 The stellar UV field strength, $\chi$, is a dimensionless quantity defined as the integral over the radiation field (91–205 nm), normalized to that of the Draine field (Draine & Bertoldi 1996).

Table 5. Modelled and slit filtered line fluxes.

| Transition | $\lambda_{\text{line}}$ [\mu m] | $F_{\text{line}}$ [10$^{-15}$ erg cm$^{-2}$ s$^{-1}$] | $F_{\text{cont}}$ [10$^{-15}$ erg cm$^{-2}$ s$^{-1}$] |
|------------|---------------------------------|---------------------------------|---------------------------------|
| (1–0)P21   | 4.8652                          | 35.22                           | 5.17                            |
| (1–0)P22   | 4.8760                          | 32.96                           | 5.14                            |
| (1–0)P26   | 4.9204                          | 28.04                           | 5.03                            |
| (1–0)P30   | 4.9668                          | 25.51                           | 4.91                            |
| (1–0)P27   | 4.9318                          | 27.23                           | 5.00                            |
| (2–1)P25   | 4.9710                          | 2.87                            | 4.90                            |
| (2–1)P21   | 4.9269                          | 2.87                            | 5.01                            |
| (2–1)P23   | 4.9490                          | 2.86                            | 4.96                            |
| (2–1)P27   | 4.9947                          | 2.94                            | 4.85                            |
| (2–1)R09   | 4.6448                          | 2.97                            | 5.81                            |
| (2–1)R10   | 4.6374                          | 3.05                            | 5.84                            |
| (2–1)R11   | 4.6301                          | 3.11                            | 5.86                            |
| (2–1)R12   | 4.6230                          | 3.20                            | 5.89                            |
| (2–1)R13   | 4.6160                          | 3.25                            | 5.92                            |
| (2–1)R14   | 4.6090                          | 3.26                            | 5.94                            |
| (2–1)R08   | 4.6523                          | 2.77                            | 5.78                            |
| (2–1)R04   | 4.6831                          | 1.98                            | 5.69                            |
| (2–1)R05   | 4.6752                          | 2.19                            | 5.70                            |
| (2–1)R06   | 4.6675                          | 2.44                            | 5.73                            |
| (3–2)P21   | 4.9901                          | 1.10                            | 4.86                            |
| (3–2)P15   | 4.9257                          | 1.14                            | 5.01                            |
| (3–2)P14   | 4.9154                          | 1.14                            | 5.04                            |
| (3–2)P11   | 4.8853                          | 1.13                            | 5.12                            |
| (3–2)P07   | 4.8468                          | 1.04                            | 5.22                            |
| (3–2)R14   | 4.6670                          | 1.30                            | 5.74                            |
| (3–2)R17   | 4.6464                          | 1.35                            | 5.81                            |
| (3–2)R18   | 4.6398                          | 1.35                            | 5.83                            |
| (3–2)R20   | 4.6268                          | 1.38                            | 5.88                            |
| (3–2)R23   | 4.6080                          | 1.41                            | 5.95                            |
| (4–3)P08   | 4.9185                          | 0.66                            | 5.03                            |
| (4–3)R29   | 4.6311                          | 0.81                            | 5.86                            |
| (4–3)R27   | 4.6425                          | 0.81                            | 5.82                            |
| (4–3)R23   | 4.6665                          | 0.80                            | 5.73                            |

Notes. With a simulated slit at position angle PA = 145° corresponding to the observed lines collected on the 29th.

the 29th cannot be explained by a single slit pointing offset of 0′′06 (the line profile at PA = 235° is leaning toward the wrong side). The middle and lower frame of Fig. 6 show that the line shape variations observed on the 30th could be explained by one single consistent pointing offset of 0′′06. Table 5 lists the line fluxes and continuum fluxes for each modelled slit filtered line.

5.4. Boltzmann plots/population diagrams

As described in the observational section, rotational diagrams are produced for the modelled line transitions for the two orthogonal position angles separately. The rotational diagrams are shown in Fig. C.1.

Adding up all $J$ levels for each $\nu$-band separately, modelled vibrational diagrams were made, following the scheme of the observed vibrational diagrams and plotted together with these in Fig. 3. We find a $T_{\nu v} = 1691$ K at PA = 145 and $T_{\nu v} = 1698$ K at PA = 55 (with the lines and observational conditions from the 29th, see Tables 1 and 2). This underestimates the corresponding observed vibrational temperature by almost a factor of two (Sect. 4.1), i.e. from our model we expect a much larger difference between line fluxes from differing $\nu$-bands than we actually observe. For the 30th we find a $T_{\nu v} = 1908$ K at PA = 10 and $T_{\nu v} = 1884$ K at PA = 100. Here, we are close to the observed values (Sect. 4.1) but the $\nu = 1$ level is not included (no
**Fig. 4.** Top: gas density distribution on the left and strength of the UV radiation field log (χ), on the right. Contour lines showing AV,rad = 1.0 (white) and min(A_V,ver, AV,rad) = 1.0 (black) are overplotted on both. Middle: gas temperature on the left and CO abundance on the right. Contour lines showing the gas temperatures of 200 K, 800 K, and 2k = 2000 K (the temperatures in the gap should reflect those in a very low density ISM medium) are overplotted on both. Lower left: the ro-vibrational bands of the CO molecule. Lower right: the modelled SED with observational data overplotted as blue dots.

High quality ν = 1 lines where detected at these PA in the observations). For completeness, a full vibrational diagram including all 60 rotational levels present in the model, was produced for each of the four vibrational levels and is shown in Fig. 7. The vibrational diagram from our modelled sample, including only lines observed on the 29th, are overplotted for comparison. We find vibrational temperatures that are similar, but the sample from the 29th has been shifted up (by a factor of 29.4) for
the presentation. In Fig. 7, we also overplot two vibrational diagrams made using fluxes from our model but line samples equivalent to that used in Brittain et al. (2009). In one we use transitions from the first four v-bands while in the other we exclude the $v = 1–0$ transitions from the fit (this approach is used in van der Plas et al., in prep.). These two were also shifted by a factor of 29.4. It is clear from this comparison that varying the sample of the CO ro-vibrational lines included in the vibrational diagram can alter the derived vibrational temperature significantly.

5.5. Line fluxes and band ratios

To further visualize our model to observation comparison, we overplot modelled and observed fluxes as a function of wavelength. We select the full line dataset collected at PA = 145° observed on the 29th (since this is the night with the best S/N and the position angle with least slit loss) (Fig. 8). The model line fluxes for the $v = 1–0$ band are within a factor of two of the observed values. The model line fluxes of the higher $v$-bands fall a factor of 10 below the observed values. Hence the line ratio between higher and lower $v$-band lines is much higher in models than in observed data.

5.6. UV fluorescence

From our model, we find that $T_{\text{rot}}$ is approximately equal to $T_{\text{vib}}$, while, from the observations we find a $T_{\text{vib}}$ which is about 2–3 times $T_{\text{rot}}$, indicating that fluorescence contributes strongly to the excitation. To assess the performance of the UV fluorescence in the model, Fig. 9 shows a line flux versus wavelength plot of the model with and without UV fluorescence. For the $v = 1–0$ lines the fluxes are similar, at $v = 2–1$ the model with UV fluorescence is about a factor of two higher and finally the higher $v$-bands are about a factor of ten higher with UV fluorescence. The vibrational temperature calculated from the fluxes without UV fluorescence is $T_{\text{vib}} = 1099$ K, while the previously derived value, for the model with UV fluorescence on was $T_{\text{vib}} = 1691$ K. The UV fluorescence has significantly improved the modelled line fluxes and line ratios but just not enough.

The model with UV fluorescence piped through the slit simulator reproduces the observed line shapes and the line flux of the $v = 1–0$ lines. However, the model underestimates the line fluxes of the remaining higher $v$-bands and the derived vibrational temperatures, indicating that the ratios of the $v$-bands with respect to one another are not correct (see Fig. 8). From our observational
data, we find band ratios around 0.2–1 for the first four vibrational bands while the model predicts band ratios of about 10/1 between the first two vibrational bands.

To explore this discrepancy in line fluxes and ratios between model and observations, we ran several models with various parameters altered. These alternative models are listed in Table 6.

The main idea in all of the tests is to get the CO warmer or exposed to more UV fluorescence. Since the gas heating/cooling and chemistry are calculated self-consistently we cannot change the position or the temperature of the CO directly but other parameters are not as constricted: 1) We increase the PAH abundance, since PAH is important in the heating of the gas. 2) We switch on CO self-shielding, since CO can then protect itself from photo dissociation by UV radiation and thereby sit higher up in the disc. 3) and 4) We increase the grid size. Most of the CO emission comes from a narrow region at the disc wall and maybe we do not resolve this region well enough. 5) and 6) We use a smaller gas to dust mass ratio. This allows us to test the effects of lower gas volume densities leading to less efficient de-population of higher levels by collision. The model that comes closest to reproduce the vibrational temperature and thereby

Fig. 6. The top four panels are the average modelled and slit filtered comparison of the line sample collected on the 29th at PA = 55/145/235/325, the middle four panels are the average modelled and slit filtered comparison of the line sample collected on the 30th at PA = 55/145/235/325 and the bottom four panels are the average modelled and slit filtered comparison of the line sample collected on the 30th at PA = 10/100/190/280. For all frames the pointing offset was 0.6′′. The black lines are the median of all the individual modelled transitions (The individual lines are all quite similar and the median therefore looks almost identical to the individual lines). The red lines are the average observed line profile (described in Sect. 4). The sample of lines plotted and used for the average are those listed in Table 2.

Fig. 7. Vibrational diagram from the modelled lines of the lowest four v levels with all 60 rotational levels included. The vibrational diagram from the modelled lines including only those in the sample observed on the 29th is overplotted. We also overplot two vibrational diagrams made using fluxes from our model but line samples equivalent to that used in Brittain et al. (2009). In one we use transitions from the first four v-bands while in the other we exclude the v = 1–0 transitions from the fit. The limited samples have been shifted by a factor of 29.4 for the presentation. The line fluxes used in this plot have not been slit filtered. Observing through a slit at various PA just shifts all the fluxes by the same constant factor and does not change the fitted $T_{vib}$ substantially.

Fig. 8. Flux versus wavelength for all lines observed on the 29th at PA = 145° listed in Table 2. The observed data is shown as triangles and for comparison the modelled fluxes are shown as stars. The different vibrational bands are colour coded: v = 1–0 is black, v = 2–1 is blue, v = 3–2 is green, and v = 4–3 is red. The error bars are in some cases within the size of the symbol.
all in rotation, but also asymmetric line profiles are observed. The file shape. Both symmetric double peaks, as expected for a disc in our sample of observed lines, we see variations in line pro-

6. Discussion

In our sample of observed lines, we see variations in line profile shape. Both symmetric double peaks, as expected for a disc in rotation, but also asymmetric line profiles are observed. The line shapes change with varying PA, but stay the same through all \( v \)-levels and rotational quantum number \( J \). Shape variations

between PA are expected because of the similar angular size of the slit width and the disc wall. Meanwhile, in the two different nights, we see different profile shapes for the same PA (PA = 235\(^\circ\)), indicating a changing offset from one night to the next. Figures A.6 and A.7 in Appendix A.2.1, visualize the changes in offsets seen from the line profile over time.

Through the first full night, where the telescope is re-centred several times, three of the four position angles are consistent with one roughly constant offset, i.e. the offset cannot be caused by a random error. The spectra from the remaining position angle would suggest a very different offset than the rest but was collected in between the rest. On the second night the various position angles could be consistent with one offset. Pointing offsets can explain the observed line shape asymmetries well, but the source of the offset is not fully understood. A test observation was recently performed with the CRIRES instrument (July 2013) observing HD 100546 at antiparallel position angles. The presence of an offset was confirmed and is most likely caused by a misalignment between slit rotation axis and the centring of the instrument. This type of misalignment can, for cases where the disc is spatially resolved (nearby discs) and the emission is com-

ing from a limited region (e.g. transitional discs), have a very large impact on the CO ro-vibrational line profiles (e.g. mimic disc asymmetries). However, for discs with no inner gap, the CO ro-vibrational lines are emitted much closer to the star and would therefore not be affected much by slit offsets. The same is true for more distant discs that are not spatially resolved.

In general, line profile asymmetries could also be explained by disc asymmetries. The line profile variations that originates from an elliptical emitting region with the star offset, would be qualitatively similar to those arising from a slit pointing offset along the semi-major axis of the disc. In that sense our grid of offset versus PA variations (Fig. A.5) can also give an indication about how disc asymmetry would a

fect the line profile

Notes. We list line fluxes and vibrational band ratios. Varied parameters are: the dust/gas mass ratio, the PAH abundance, the grid size and switching CO self shielding on/off. The outcome of the various models (without slit filtering applied) are presented here by comparison of the \( T_{\text{vib}} \) and the line flux for two representative lines: \( v(2-1)\text{R06}, v(1-0)\text{P22} \). All model here are unfiltered. The line sample used for the computation of \( T_{\text{vib}} \) is that collected on the 29th and the observational result is shown at the top.

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ing from a limited region (e.g. transitional discs), have a very large impact on the CO ro-vibrational line profiles (e.g. mimic disc asymmetries). However, for discs with no inner gap, the CO ro-vibrational lines are emitted much closer to the star and would therefore not be affected much by slit offsets. The same is true for more distant discs that are not spatially resolved.

In general, line profile asymmetries could also be explained by disc asymmetries. The line profile variations that originates from an elliptical emitting region with the star offset, would be qualitatively similar to those arising from a slit pointing offset along the semi-major axis of the disc. In that sense our grid of offset versus PA variations (Fig. A.5) can also give an indication about how disc asymmetry would affect the line profile shapes. However, in this case the “offsets” derived from the line profiles should not change between various position angles or from one night to the next, but rather indicate the same offset. One could imagine that the disc could have an uneven distribution of CO emitting regions. To explain asymmetric variations between all position angles, we could have several randomly distributed strong CO emitting “spots” that by chance fall into some of the position angles. Even in this case, we should not
see changes from one night to the next at the same PA, or anti-parallel PA. This would imply that the disc has undergone some physical change between such varying spectra. This kind of change is highly unlikely since the time between collection of spectra is too short for variations in the disc to happen (down to 20 min).

Brittain et al. (2013) found single peaked profiles for the CO ro-vibrational emission from HD 100546. They use the Gemini South telescope with a slit width of 0.34″. The double-peaked shape could be lost due to their lower spectral resolution ($R = 50000$). Comparing several observations at different epochs, they find a small shifting asymmetry only present in the $v = 1–0$ lines. They suggest this could be due to a circumplanetary CO component orbiting in the outer disc. According to their analysis, this additional CO component would be at zero velocity at the epoch of our observations (Brittain, priv. comm.). With our very narrow slit, the small CO component would easily be filtered out, meaning that our symmetric double peaked line profiles and the above conclusions are not inconsistent with their findings.

The sensitivity of the line profile shape to slit PA changes indicates that the main contribution to the CO ro-vibrational emission is coming from the disc wall. The shapes of the observed lines are similar for all $v$-levels, also supporting that these lines should all originate in the same region (the disc wall). The model prediction that most of the emission originates between 10 and 13 AU, is consistent with this. Our modelled spatial extent underestimates the observed as found by Goto et al. (2012) by a factor of 0.7. However, the modelled extent was calculated from one line while the observed was calculated from a range of $v = 2–1$ lines. Furthermore, the comparison needs to be improved by convolving the modelled spatial profile with the observed PSF instead of just approximating by a Gaussian and by co-adding the same sets of lines (work in progress).

Measuring line fluxes and flux ratios (vibrational temperatures), there are inconsistencies between model and observations. Our model line fluxes are consistent with observations within a factor of two for the first vibrational band. We underestimate the line fluxes of the higher $v$-bands by about a factor of ten. We therefore also underestimate the line flux ratios by up to a factor of ten. This is probably because the CO is not sufficiently pumped by UV fluorescence. At heights in the disc where the stellar UV field reaches directly, CO self-shielding and H$_2$ shielding play a minor role.

We can reproduce the line flux ratios from the observations with lower gas volume densities, potentially connected to the inner rim. We checked that the scale height calculated from the gas temperature is not significantly different from what the input in the parameterized model. A low velocity disc wind as a cause for a low density vertically extended CO component can be ruled out since Pontoppidan et al. (2008) and Bast et al. (2011) showed that this would cause single-peaked instead of double-peaked line profiles.

7. Conclusion

In this paper, we present for the first time an extensive analysis of a large comprehensive set of observational data of the CO ro-vibrational emission lines from the disc around HD 100546: Collected at eight different position angles covering six different grating settings at the CRIRES/VLT. The observations show line asymmetries and the line profile shapes vary with position angle. We also present modelled emission lines, using a ProDiMo model of HD 100546 piped through a slit filtering tool. This model is in no way designed for the CO ro-vibrational lines, so the model produces the observed as well, confirming our very narrow slit, the small CO component would easily be filtered out, meaning that our symmetric double peaked line profiles and the above conclusions are not inconsistent with their findings.

The sensitivity of the line profile shape to slit PA changes indicates that the main contribution to the CO ro-vibrational emission is coming from the disc wall. The shapes of the observed lines are similar for all $v$-levels, also supporting that these lines should all originate in the same region (the disc wall). The model prediction that most of the emission originates between 10 and 13 AU, is consistent with this. Our modelled spatial extent underestimates the observed as found by Goto et al. (2012) by a factor of 0.7. However, the modelled extent was calculated from one line while the observed was calculated from a range of $v = 2–1$ lines. Furthermore, the comparison needs to be improved by convolving the modelled spatial profile with the observed PSF instead of just approximating by a Gaussian and by co-adding the same sets of lines (work in progress).

Measuring line fluxes and flux ratios (vibrational temperatures), there are inconsistencies between model and observations. Our model line fluxes are consistent with observations within a factor of two for the first vibrational band. We underestimate the line fluxes of the higher $v$-bands by about a factor of ten. We therefore also underestimate the line flux ratios by up to a factor of ten. This is probably because the CO is not sufficiently pumped by UV fluorescence. At heights in the disc where the stellar UV field reaches directly, CO self-shielding and H$_2$ shielding play a minor role.

We can reproduce the line flux ratios from the observations with lower gas volume densities, potentially connected to the inner rim. We checked that the scale height calculated from the gas temperature is not significantly different from what the input in the parameterized model. A low velocity disc wind as a cause for a low density vertically extended CO component can be ruled out since Pontoppidan et al. (2008) and Bast et al. (2011) showed that this would cause single-peaked instead of double-peaked line profiles.

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Appendix A: Line profiles and slit loss

In our dataset, we found clear variations in the shape of line profiles observed at different position angles. These variations are due to the relative size of the slit and the disc on the sky (Fig. 1). At the distance of HD 100546 (103 pc), a slit width of 0.‘2 corresponds to a width of about 20 AU. This is coincidently close to the diameter of the disc wall. Figure 1 shows how varying the position angle of the slit results in losing parts of the emission originating at the disc wall (10–13 AU). Thus different slit position angles will lead to different profile shapes. For HD 100546 the resulting line profiles show double peaks at PA = 145° and PA = 325°, while showing flat topped profiles at PA = 55° and PA = 235°.

With a slit width that barely includes most of the disc wall, a poorly centred slit can affect the shape of the lines. If the slit is offset to one side, we lose emission from the velocity channels falling outside the slit. These important effects need to be considered in both our observational analysis and in our modelling efforts.

A.1. Observed line profiles

Table 2 presents a full listing of our selected unblended and clean CO ro-vibrational lines. For all these CO ro-vibrational transitions, line profiles (flux as a function of velocity) have been extracted. To investigate whether we can build high resolution average line profiles, we checked the data for shape variations as a function of \( v, J, \) and different nights.

The individual line profiles are normalized by their fitted continuum, shifted to zero continuum, and the line profile is then normalized to the maximum flux value. Profiles are then combined to median average profiles.

The profile shapes vary between the two nights and also between the four/eight different position angles. We find no significant variations when comparing \( v \)-levels and wavelength settings (see Fig. A.1 for an example at PA = 145° for the night of the 29th). For a more quantitative view, the FWHM and the peak separations, \( \sigma_\text{sep} \), for PA = 145° are shown for all \( v \)-bands in Table A.1. The average for each \( v \)-band is build over the individual \( J \) transitions at that \( v \)-band. The 1\( \sigma \) standard deviation listed in the table is the deviation of the values at each \( J \)-level from the mean. The average from all \( v \)-bands agree with each other within 1\( \sigma \).

The difference between line shapes observed at the same PA on the 29th and on the 30th could be explained by different pointing offsets present for each night. Within the individual position angles there are no shape variations during one night, i.e. data from different wavelength settings taken at different times with same PA are very similar.

The above found stability of the line profile shapes justifies building averaged line profiles over velocity for each PA and each night (independent of \( v, J \)). These co-added line profiles are shown in Fig. A.2. For the 29th, we find double peaked profiles at both PA = 145° and PA = 325°, as we would expect given the disc itself has a position angle of 145°. At PA = 55° and PA = 235°, we find single peaked asymmetric profiles, indicating an offset (with no offset we should find flat topped profiles). The profiles for the anti-parallel positions PA = 55° and PA = 235°, though very similar, do not match exactly but lean in opposite directions, which should not be the case for a true antiparallel case. For the 30th, the four repeated position angles (PA = 55°, PA = 235°, PA = 145°, and PA = 325°) show slightly altered shapes indicating a change in the offset with respect to the first night. The four new position angles (PA = 10°, PA = 190°, PA = 100°, and PA = 280°) all show asymmetric single peaks with a hint of a shoulder.

Table A.1. FWHM and peak separation of the average line profiles.

| \( v \)-band | FWHM [km s\(^{-1}\)] | \( \sigma \) | \( \sigma_\text{sep} \) [km s\(^{-1}\)] | \( \sigma \) |
|-------------|---------------------|-----|-----------------|-----|
| \( v = 1-0 \) | 18.30 | 1.05 | 10.70 | 0.57 |
| \( v = 2-1 \) | 18.16 | 0.76 | 10.50 | 2.47 |
| \( v = 3-2 \) | 18.25 | 0.68 | 11.97 | 1.34 |
| \( v = 4-3 \) | 18.35 | 0.64 | 11.14 | 2.10 |

Notes. Done for each \( v \)-band separately for lines observed at the PA = 145° on the 29th. The error listed is the 1\( \sigma \) standard deviation of the individual \( J \)-levels included in each average.

A.2. Modelled line profiles

ProDiMo outputs line data cubes for each chosen CO ro-vibrational transition. Each cube contains a \( 201 \times 201 \) pixel coordinate grid in units of AU and the spectral intensity in \([\text{erg/cm}^2/\text{s/Hz/sr}]\) at every spatial position in the described coordinate grid for each of the 91 velocity channels, covering \(-20 \text{ km s}^{-1}\) to \(+20 \text{ km s}^{-1}\) and the continuum (see Appendix B). From this cube we create line images, profiles, and flux tables. They are our modelled “observations”.

A.2.1. Applying a slit filter to line data cubes

The line cubes do not contain any observational or instrumental effects. Hence, they need to be convolved with the instrumental PSF (we approximate the PSF by a Gaussian), rotated to the position angle of the disc on the sky and corrected for slit loss and pointing offsets before comparison with the actual observations. Each cube is therefore piped through a slit filtering IDL procedure (Carmona et al. 2011) adapted for the purposes in this paper. The slit filter applies the described corrections and produces line profiles that can be directly compared to our observed data.

Each spectral slice of the ProDiMo data cube is convolved in the spatial \((x, y)\) direction with a Gaussian two dimensional PSF
Fig. A.2. Averaged line profiles at eight different position angles containing transitions from all \( v \)-levels observed on the 29th and 30th, listed in Table 2. The dotted lines are the normalized individual transitions and the red line is the median of all these lines. The upper four panels show the line profiles collected at PA = 55°/145°/235°/325° on the 29th. The middle four panels show the line profiles collected at PA = 55°/145°/235°/325° on the 30th. The lower four panels show the line profiles collected at PA = 10°/100°/190°/280° on the 30th.

Each spectral slice of the data cube is now covered with a two dimensional mask \((x, y)\) representing the spectrograph slit (with arbitrary orientation and/or offset from the disc centre and centred on \(x_0\), slit, \(y_0\), slit). From the resulting signal we calculate the line profile and astrometric signal (SPP and FWHM). The SPP is calculated as the shortest distance between the centre of mass (centroid) of the CO + continuum emission and a line perpendicular to the slit running through the slit origin. The FWHM is calculated from a Gaussian fit to the CO + continuum emission. Figure A.3, shows for three different offsets the effect that slit filtering has on a line profile, together with a sketch of

![Fig. A.3](image-url)
Flux versus wavelength comparing the slit filtered model to the non slit filtered model for all lines observed on the 29th at PA = 145° listed in Table 2. The slit filtered modelled fluxes are shown as diamonds and the modelled fluxes without slit filter are shown as stars. The different vibrational bands are colour coded: $v_{1}=1$–0 is black, $v_{2}=2$–1 is blue, $v_{3}=3$–2 is green and $v_{4}=4$–3 is red.

The slit on disc. The line profiles are normalized in the same way as the observed profiles (see Sect. A.1).

To assess the importance of slit loss and telescope effects, we have also compared the unfiltered model line fluxes to the slit filtered model line fluxes (Fig. A.4). We find that the slit affects all transitions in the same way and flux ratios are conserved through the slit filtering. This was expected, because the spatial profiles of the line emission are very similar.

Because our observed line profiles change on very short time scales (see Appendix A.1) it is virtually impossible to explain the shape asymmetries and variations with disc asymmetries alone and this calls for the shape variations to be caused by pointing offsets.

To explore the variety in line profiles due to varying PA and pointing offsets, we select a representative line, $\alpha(2\text{--}1)$R06, and study seven different offsets ($-0\farcs20; -0\farcs15; -0\farcs10; -0\farcs06; -0\farcs03; 0\farcs10; 0\farcs20$), measured along the semi-major axis of the disc (positive to the right) while varying the slit position angle from 15° to 175° with a step size of 10°. The full parameter grid of line profile shapes is presented in Fig. A.5. These tests show that the shape variations seen in our observed data are fully consistent with the variations from a combination of PA and/or offset covered in our theoretical grid. From our theoretical grid we furthermore derive the plots shown in Figs. A.6 and A.7. Here the pointing offsets needed to explain our observed line profile variations are plotted as a function of Time and PA these figures reveal that a pointing offset of $-0\farcs06$ would be an appropriate assumption for most position angles. This offset was imposed on the slit filtering procedure for the simulated lines of the night of the 29th and 30th. For our full selection of lines the slit filtering procedure is run for various position angles based on the settings and the PSF of the observations made on the 29th and 30th of March 2010, listed in Table 1.

For comparison purposes, the final modelled line profiles are normalized co-added and averaged for each PA setting separately, following the exact same scheme as the combining of the observed line profiles (see Appendix A.1 for more details). These normalized combined line profiles are shown in Fig. 6 with the corresponding average observed line profiles over-plotted. Table 5 lists the line fluxes and continuum fluxes for each modelled slit filtered line at one particular position angle (PA = 145°).

The upper frame of Fig. 6 shows that the line shape variations, that we see in our observations from the 29th, cannot be explained well by a single slit pointing offset of $-0\farcs06$ (the line profile collected at PA = 235° is leaning toward the wrong side). The middle and lower frame of Fig. 6 show that the line shape variations observed on the 30th could in principle be explained by one single consistent pointing offset. The slit filtered model (with a pointing offset of $-0\farcs6$) reproduces the observed line shapes reasonably well.
Fig. A.5. Parameter exploration made with our slit filtering tool. The position angle of the slit was varied from 0° to 175° in steps of 10°. The offset values are –0′′20, –0′′15, –0′′10, –0′′06, –0′′03, 0′′, 0′′10, and 0′′20. The slit position angle is varied when moving horizontally in the figure (the PA values are printed at the top) and the offset is varied when moving vertically in the figure (the offset values are printed on the left). The y values are normalized fluxes from –0.1 to 1.7, while the x values are velocities from –15 km s$^{-1}$ to +15 km s$^{-1}$. 

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Appendix B: A flux-conserving scheme to convert images in polar coordinates to regular Cartesian grids

Continuum images and channel maps in ProDiMo are initially calculated on a polar grid (see Thi et al. 2011 for details) with roughly logarithmic equidistant radial grid points \( r_i \) \( i \in [0...N_r] \) and linear equidistant angular grid points \( \theta_j \) \( j \in [0...N_\theta] \). This is necessary to resolve the tiny inner disc rim (important for the short wavelengths) as well as resolving the outer regions (important for the long wavelengths) at the same time.

The polar intensities \( I_i(r, \theta) \) have associated areas in the image plane as

\[
A_i = \pi (r_i^2 - r_{i-1}^2)/N_\theta \quad \text{for} \quad i \in [1...N_r], \quad j \in [1...N_\theta]. \tag{B.1}
\]

The intensities are assumed to be constant on the polar “pixels”, i.e. the area \( A_i \) bracketed by \( r_i, r_{i-1}, \theta_j \) and \( \theta_{j-1} \), see Fig. B.1.

We seek a fast numerical method to convert these polar images onto a regular grid with equidistant Cartesian image coordinates \( (x_n, n \in [0...N_x]) \) and \( (y_k, k \in [0...N_y]) \) with associated pixel areas

\[
A_{nk} = (x_n - x_{n-1})(y_k - y_{k-1}) \quad \text{for} \quad n \in [1...N_x], \quad k \in [1...N_y]. \tag{B.2}
\]

\( ^2 \) Some adjustments inside the inner rim and increased resolution towards the outer disc radius and beyond.

The method is flux-conservative if

\[
\sum_{i=1}^{N_r} \sum_{j=1}^{N_\theta} A_{ij} I_i(n, j) = \sum_{n=1}^{N_r} \sum_{k=1}^{N_\theta} A_{nk} I'_n(n, k) \tag{B.3}
\]

where \( I'_n(n, k) \) are the desired intensities on the regular Cartesian pixels. The exact solution of this problem would be to calculate the overlap areas, \( O(A_{nk}, A_{ij}) \), between the regular pixels \( A_{nk} \) and any polar pixel \( A_{ij} \), then sum up the fluxes and divide by the pixel area as

\[
I'_n(n, k) = \sum_{i=1}^{N_r} \sum_{j=1}^{N_\theta} O(A_{nk}, A_{ij}) I_i(n, j), \tag{B.4}
\]

but to calculate those overlap areas is painful, see Fig. B.1. A more practical idea is to create a Cartesian rectangular area that exactly contains the polar pixel, see Fig. B.1. by taking the minimum and maximum of the four corner points of \( A_{ij} \)

\[
x_j = \min(x_{ij}, x_{i-1j}, x_{ij}, x_{ij}), \quad y_j = \min(y_{ij}, y_{ij}, y_{ij}, y_{ij}),
\]

\[
x_i = \max(x_{ij}, x_{ij}, x_{ij}, x_{ij}), \quad y_i = \max(y_{ij}, y_{ij}, y_{ij}, y_{ij}),
\]

\[
x_j = r_{i-1} \sin(\theta_j), \quad y_j = r_i \cos(\theta_j),
\]

\[
x_j = r_{i-1} \sin(\theta_j), \quad y_j = r_i \cos(\theta_j),
\]

\[
x_j = r_{i-1} \sin(\theta_j), \quad y_j = r_i \cos(\theta_j).
\]

The area of this rectangular pixel,

\[
A'_{ij} = (x_j - x_i)(y_j - y_i),
\]

is always larger than the area of the original polar pixel \( A_{ij} \), resulting in a correction factor in Eq. (B.7) below. The area overlaps between \( A_{nk} \) and \( A'_{ij} \) are now easy to calculate, and the resulting conversion formula is

\[
C_{nk} = \sum_{i=1}^{N_r} \sum_{j=1}^{N_\theta} O(A_{nk}, A'_{ij}) A_{ij}/A'_{ij}
\]

\[
I'_n(n, k) = \frac{1}{C_{nk}} \sum_{i=1}^{N_r} \sum_{j=1}^{N_\theta} O(A_{nk}, A'_{ij}) A_{ij}/A'_{ij} I_i(n, j). \tag{B.7}
\]
Fig. B.2. Rotational diagram for each of the first four $v$ levels made from observational data gathered on the 29th. In each plot, data from two position angles are plotted for comparison (PA = 55° shown as red squares and PA = 145° shown as blue triangles). A linear fit to find $T_{\text{rot}}$ is made separately for each PA. The fitted values are printed on the plots together with their formal error bars. However, we expect a somewhat larger error from the limited $J$ range.

Fig. B.3. Rotational diagram for each of the first four $v$ levels made from observational data gathered on the 30th. In each plot, data from two position angles are plotted for comparison (PA = 55° shown as red squares and PA = 145° shown as blue triangles). A linear fit to find $T_{\text{rot}}$ is made separately for each PA. The fit is strongly affected by the limited line sample. To visualize this effect the rotational diagrams from the 29th are overplotted in black.
Appendix C: Population diagrams

C.1. Observed rotational diagrams

Rotational diagrams were compiled, for each vibrational level, using the integrated line fluxes derived from the CRIRES data separating data from different position angles and observing nights. We note that in our sample the most optically thick lines, like the \( v = 1-0 \) low \( J \) lines, are missing (these lines coincide with strong telluric absorption features and are therefore excluded). The rotational diagrams are shown in Figs. B.2 and B.3. The details of the equations and quantities used are described in Sect. 4.1. We see that there is no big variation between the fit for two position angles taken on the same night. The rotational temperatures found from each of the two observing nights are different, but this is mainly caused by a narrower fitting range in \( J \) levels for the second night. The \( v = 2-1 \) and \( v = 4-3 \) rotational diagrams are to sparsely populated and no \( v = 1-0 \) lines were collected in the second night. For the first observing night the \( v = 2-1 \) rotational diagram shows a \( T_{\text{rot}} \sim 1100 \) K and the \( v = 3-2 \) rotational diagram shows a \( T_{\text{rot}} \sim 1300 \) K. And for the second night the \( v = 3-2 \) rotational diagram shows a \( T_{\text{rot}} \sim 1100/1200 \) K. In these diagrams, the individual lines all fall on a curve typically seen in the presence of optical depth and non-LTE effects, making a linear fit questionable. Thi et al. (2013) showed that it is hard to fit a single temperature and that the real rotational temperature can be found in a “second” turn over at higher \( J \) levels. We do not have a wide enough \( J \) range for this. The formal error bars for the rotational temperatures are printed on the rotational diagrams but we expect that there is a somewhat larger error from the limited \( J \) range.

C.2. Modelled rotational diagrams

As described for the observational data, rotational diagrams were produced for the modelled line transitions (comparable to the data collected on the 29th) for two orthogonal position angles separately. The rotational diagrams are shown in Fig. C.1 and the details of derivations are described in Sect. 4.1. The rotational temperatures found from the modelled lines are higher than those observed, but the lines fall on a curve and it is hard to get a good linear fit. The fit depends heavily on the range of lines included.

Fig. C.1. Rotational diagram of the lowest four \( v \) levels for the modelled line sample. The fitting is done with the exact same range and line selection as the observational data set collected on the 29th, see Table 2.