Abstract

Spectra containing CO ro-vibrational emission lines from HD 163296 observed at different epochs are not fully consistent with each other. The line shapes and the FWHM (Full Width Half Maximum) do not agree. Variations in NIR brightness have been reported and could be linked to these differences. The aim of this chapter is to explore the cause of the difference in line profile shape observed over more than a decade. Furthermore, we wish to understand the single peaked line profile appearance in the most recently collected data set versus the earlier reported double-peaked appearance. The thorough study of this disc will improve our understanding of the correlation between CO ro-vibrational transition line shape and inner disc geometry. We derive values for FWHM, line fluxes and peak separation (where relevant) for the CO ro-vibrational lines from the two separately collected data sets. The FWHM (Full Width Half Maximum) of the median compiled from observations are 10-25 km/s larger in the earlier epoch, and confirmed double peaks are only present in high $J$ lines from the early epoch. FWZI (Full Width Zero Intensity) values are similar in both epochs making an additional central component in the later epoch a likely explanation for the single peaks and the lower FWHM. We use the thermo chemical disc code ProDiMo to calculate modelled CO ro-vibrational lines from a previously published model of this source and compare the line shapes, peak separations, FWHM, and line fluxes, to those observed. The ProDiMo model reproduces the FWHM, the peak separations, and the line fluxes of the high $J$ lines from the earlier epoch well. For the remaining lines FWHM are over predicted and line fluxes are under predicted by a factor ~2.
We propose that a variable non-Keplerian component of the CO ro-vibrational emission is present in both data sets, but with a stronger contribution in the most recent data set. Further observations are needed to confirm the variability, e.g. additional CO ro-vibrational line detections (with CRIRES/VLT or NIRSPEC/Keck) or Ne II line observations with VISIR/VLT. From both observed and modelled line fluxes we derive Boltzmann diagrams with various $J$ coverage, to asses how reliable the slope of these diagrams can estimate the gas temperature in the line emitting region. We find a high level of degeneracy in the fitted temperatures due to the limitations in LTE (local thermodynamic equilibrium), single temperature, slab models. We suggest that these diagrams should be used mainly in a comparative manner, between observations with the same $J$ coverage or comparing observations with detailed disc models.

4.1 Introduction

Herbig Ae/Be (HAeBe) stars are intermediate mass pre main sequence stars that are surrounded by discs. CO ro-vibrational emission is frequently observed from these discs (Blake & Boogert 2004, Brittain et al. 2007, 2009, van der Plas et al. 2009) and traces the inner regions close to the star, where planet formation is expected to occur.

When observing emission lines from discs around Herbig stars, the shape of the line profiles can reveal important information about the geometry of the emitting gas. However, observed line shapes are not only a product of the physics and geometry in the discs, but observational conditions and instrumental effects will also distort line profile shapes in the following ways: Low signal to noise can create asymmetric profiles or add double peaks to a flat topped profile, low spectral resolution can smoothen out double peaks or multiple component features, and observations through slits can cut away parts of the velocity field when observing spatially resolved emission (Hein Bertelsen et al. 2014, Chapter 2). Because of this, observations of the same source in the same wavelength region with different instruments can be very valuable for the interpretation of the line profile shapes. As one example, the instrumental settings can in this way be identified or excluded as the cause of unexpected line profile shapes.

Emission lines from protoplanetary discs are generally expected to show double peaked profiles due to the Keplerian rotation. However, single peaked or otherwise non-Keplerian emission lines are frequently observed (Brown et al. 2013). Excluding instrumental causes, single peaked profiles can arise due to low inclination of the disc, composite emission e.g. from both the inner and outer disc, or disc winds/outflows. Disc wind scenarios includes, thermally launched winds, magnetically launched winds and funnel flows (Pontoppidan et al. 2011, Bast et al. 2011, Najita et al. 2003). Thermally launched winds are linked to irradiation by FUV (far-ultraviolet), EUV (extreme-ultraviolet), or X-ray photons. The radiation heats the upper layers of the disc causing the thermal energy to exceed the gravita-
ional potential leading to a gas flow off the disc surface (Alexander 2008, Gorti & Hollenbach 2009). Magnetic fields of classical T Tauri stars have torques thought to be large enough to launch strong winds, some with velocities around 250 km/s and some with lower velocities up to 50 km/s (Edwards et al. 2006). This was seen in the He$^1$ 10830 Å and in forbidden lines like [O i] 6300 Å. Lastly, emission lines due to the accretion from the disc onto the star through a funnel flow, may be present at the locations where the funnel flow connects to the disc. Najita et al. (2003) showed that these funnel flows would cause double peaked lines, thus they are not candidates to produce single peaked CO fundamental line emission.

CO ro-vibrational emission from disc winds has been observed (Bast et al. 2011, Pontoppidan et al. 2011). Bast et al. (2011) identified 8 T Tauri discs displaying narrow symmetric, single peaked and broad based emission lines that could not be explained by a standard Keplerian model but are instead likely due to disc winds. The authors exclude magnetic winds, due to the low velocity shifts of the lines, and funnel flows, due to the single peaked shape of the lines. The authors conclude that the lines might be a combination of emission from the warm surface seen as a broad Keplerian component, and a disc wind driven by EUV radiation or soft X-rays seen as a narrow component.

HD 163296 is a well studied Herbig Ae star of spectral type A3Ve (Gray & Corbally 1998) located at a distance of 118.6 pc (Hipparcos). It has been labeled a group II source (flat disc) by Meeus et al. (2001) and the stellar mass of the system has been estimated to $M_\star \sim 2.3 \, M_\odot$ (Montesinos et al. 2009). Using spatially resolved sub-mm data, the inclination of the disc has been estimated to $46 \degree \pm 4 \degree$ and the position angle to $128 \degree \pm 4 \degree$ (Isella et al. 2007). The disc has been studied through interferometric observations of both continuum and CO emission lines (0.87-7.0 mm) (Isella et al. 2007). From the line emission the authors found the $^{12}$CO and $^{13}$CO to be optically thick and derive an outer radius from the CO lines of 550±50 au. The continuum dust emission implies an outer radius of 200±15 au. Thus, a sharp drop in continuum emission of a factor $>30$ at a radius of 200 au, was invoked to explain the lack of continuum emission from radii larger than 200 au (Isella et al. 2007).

Tilling et al. (2012) presented Herschel/PACS observations of the disc, and used the line detections from this dataset together with additional line and continuum data to fit a ProDiMo (Woitke et al. 2009) model, in an attempt to determine disc properties. Parameter degeneracies prohibited a clear derivation of the disc properties and the authors concluded that a single disc model could not be found to fit perfectly the entire wealth of observational data for this object.

ALMA observations (band 7, $\sim 850$ μm) has put the outer dust disc radius at 240 au and the CO outer radius at 575 au (de Gregorio-Monsalvo et al. 2013). A well resolved dusty disc was seen with no indications of gaps or holes beyond 25 au. de Gregorio-Monsalvo et al. (2013) conclude that a standard tapered-edge model with one unique density profile cannot match both data sets at once. The CO channel maps require a thicker gas disc, while the mid- and far-infrared SED
require a flatter dust disc than previously presented in Tilling et al. (2012).
CO ro-vibrational \(v=1-0\) emission lines from this disc have been studied on several occasions (Blake & Boogert 2004, Salyk et al. 2011, Brittain et al. 2007, Chapter 3, from hereon B14). In Salyk et al. (2011), using NIRSPEC data from the Keck telescope, the authors identified double peaked profiles and FWHM\(\sim 83\) km/s (for \(J>25\)) indicating that the origin of the emission is close to the star. Assuming Keplerian rotation, the peak separation measured from the high J profiles would suggest an outer radius for the emission of 2-3 au. Recently, we have collected spectra containing CO ro-vibrational emission lines with CRIRES at the VLT, and found single peaked profiles for low J lines while high J lines displayed asymmetric flat topped profiles (B14). Furthermore, significantly narrower lines were found than those seen by Salyk et al. (2009), FWHM\(\sim 59\) km/s (for \(J>20\)). We will clarify in this chapter whether this is due to a physical variability of the disc or to instrumental differences.

In coronagraphic images a bipolar jet (HH 409) has been seen (Grady et al. 2000), with radial velocities for the gas in the jet of 200-300 km/s. HD 163296 has shown variations in NIR (Near Infra Red) brightness (over 30\% in \(J\)-band, 20\% at \(H\)-band, and 15\% at \(K\)-band, de Winter et al. 2001) on timescales of years (Sitko et al. 2008). This was seen as an outburst in the 1-5 \(\mu\)m wavelength region during 2002. This wavelength region corresponds to a hump frequently seen in SEDs of many HAeBes and is thought to be related to the inner wall of the dust disc. The authors found no SED model (based on data from one epoch) that could explain the full nature of this source.

Ellerbroek et al. (2014) matched transient optical fading with the enhanced NIR excess (also noticed by Sitko et al. 2008) and relate these to the jet (HH 409). The authors suggest a scenario where dust clouds, that are launched above the disc plane to heights where they cross the observers line of sight to the star, are responsible for the optical and NIR variability. Ellerbroek et al. (2014) derive a period of 16.0\(\pm 0.7\) years for the increased outflow activity from the jet. Due to epoch-sparsity of the photometric data, it could not be confirmed whether the jet period matches the NIR and optical variations, and thereby that a single mechanism is in fact responsible for both jet and photometric variability. The time elapsed between the latest CO ro-vibrational data set from HD 163296, B14, collected in 2012, and the earlier S11/B07 collected in 2001/2002 is \(\sim 10\) yr. Photometric changes for the discs have taken place during this time. Thus, any differences in the CO profiles between these data sets could be related to physical changes in the disc connected to the jet. Klaassen et al. (2013) reported the detection of a rotating molecular disc wind that extends to more than 10\"., seen from ALMA observations of the CO \(J=2-1\) and \(J=3-2\) lines. This disc wind should contain low velocity material launched from the disc at radii of a few au with velocities \(<25\) km/s. These radii and velocity channels are indeed relevant for the detected CO ro-vibrational lines and variations in these lines could therefore relate to this molecular wind.

In this paper we will make a thorough comparison to clarify the cause for these differences. Firstly we present the three sets of observational data, and the results
4.2 Observational data

We have collected high resolution spectra (R~100,000) of HD 163296 in March 2012 with the VLT cryogenic high-resolution infrared echelle spectrograph (CRIRES Kaeufl et al. 2004). These observations cover a wavelength range from 4.5 µm to 5 µm with 6 different grating settings (4.6575, 4.7363, 4.9948, 4.6376, 4.8219, and 5.0087 µm) (B14). The science data were reduced using version 2.2.1 of the CRIRES data reduction pipeline\(^1\) and telluric correction was performed by use of collected telluric standard spectra. Since the removal of telluric lines can be challenging leaving many residuals, precautions were taken to diminish these problems already during the planning of the observations. The observation dates were chosen on the basis of when the highest possible velocity shift occurred, so as to shift telluric lines away from the line profile. Low transmission regions (60-80%) were left out of the final spectrum, leaving gaps on the right wing of a few of the line profiles (see left frame of Fig. 4.2). The details of the data reduction and flux calibration can be found in B14. From this dataset, we include lines from \(J=0\) up to \(J=37\).

For comparison we have obtained another high resolution spectrum (R~25000) of HD 163296 collected with NIRSPEC (McLean et al. 1998) on the Keck II telescope. These observations are collected during the period 2001-2002. The spectra from different epochs were combined, resulting in one single spectrum per wavelength region. Low transmission regions (60-80%) were left out of the final spectrum, causing several transitions to have gaps in the centre of their line profiles (see middle frame of Fig. 4.2). The observations span a wavelength range from \(~4.65-5.15\) µm and include lines from \(J=1\) up to \(J=37\). Details on data acquisition and reduction can be found in Salyk et al. (2011, 2009) and Blake & Boogert (2004) (from here on Salyk et al. (2011) will be denoted S11).

We also included additional spectra from NIRSPEC on the Keck II telescope, obtained in March 2002. The observations span a wavelength region from \(~4.64-5.02\) µm and include lines from \(J=1\) up to \(J=33\). However, this dataset has several

\(^1\) http://www.eso.org/pipelines/
lines distorted by telluric over-correction, due to variable telluric water lines on
the night of observations. The data reduction can be found in Brittain et al. (2007)
(from here on B07).

In B14 we found a continuum flux (at \(4.770\ \mu m\)) of 16.3 Jy. For CRIRES spec-
tra, we can expect the accuracy of the flux calibration to be around \(\sim 30\%\) (Brown
et al. 2013), due to differences in width of the PSF (Point Spread Function) for the
science versus the telluric standard spectra (these differences are expected to be
due to variations in the performance of the AO system). From the S11 spectrum
a continuum flux (at \(4.770\ \mu m\)) of 12.1 Jy was found. An error of 10-20% is ex-
pected. The continuum fluxes measured in B14 and S11 are consistent within the
uncertainties. For B07, we do not have flux calibrated spectra.

### 4.3 Observational results

The individual lines collected from the three observational datasets are shown in
Fig 4.2. For the CRIRES data the spectral resolution is \(R = 100\,000\), corresponding
to \(\Delta v = 3\ \text{km/s}\), while for NIRSPEC it is \(R = 25\,000\), corresponding to \(\Delta v = 12\ \text{km/s}\).
The lines displayed in Fig 4.2 have smaller spacing between velocity channels than
the \(\Delta v = 3\ \text{km/s}\) and \(\Delta v = 12\ \text{km/s}\) mentioned above (B14 has \(\sim 1.5\ \text{km/s}\), S11 has \(\sim 4\ \text{km/s}\), and B07 has \(\sim 5\ \text{km/s}\)) due to fine sampling of the spectral resolution. In Fig. 4.3, we show normalised line profiles compiled from co-adding either all lines, all
low \(J\) lines (\(J<10\)), all mid \(J\) lines (\(10<J<20\)), or all high \(J\) lines (\(J>20\)), in separate
medians for B14, S11 and B07.

The spectrum from B14 shows single peaked emission lines for low and mid
\(J\) values while flat topped asymmetric profiles with shoulders seem to be present
at higher \(J\). The spectrum from S11 shows single peaked emission lines for low
\(J\), while mid and high \(J\) lines show either double peaked or flat topped profiles.
However, the central dips in the double peaked profiles are comparable to the
noise, and many double peaked profiles have central gaps in the spectra, where
low transmission regions due to strong telluric absorption occurred (Fig. 4.2).
4.3 Observational results

Even line profiles that display what looks like the normal central dip of a Keplerian profile could in fact be affected by telluric residuals that mimic the typical shape. Hence, the double peaked nature is uncertain for low and mid $J$ lines. High $J$ lines however, are unlikely to be affected heavily by telluric absorption, and are therefore more reliable. The spectrum from B07 shows a general mix between single peaked and double peaked emission lines with no clear connection with high or low $J$. Also, several lines suffer from telluric overcorrection giving irregular lines. Again, the central dip is mostly comparable to the noise and a single peaked nature cannot be ruled out from this dataset either. CRIRES has higher spectral resolution than NIRSPEC, and the data from B14 have many high signal to noise lines. Hence, if present at the time of observation, the double peak should have been visible in this spectrum. However, the B14 dataset has been collected a decade later than the other two datasets, thus we cannot exclude that variability may play a role. Variability has been noted for this source in the near-IR continuum and in the optical (Sitko et al. 2008, Ellerbroek et al. 2014). For these studies observations collected at several different epochs were used dating from 1979 until 2012. During this time the NIR brightness was increased by more than 10% (in $H$-.
Figure 4.2 – Individual line profiles and median at the bottom from all three datasets. Left: Line profiles from B14. Middle: Line profiles from S11. Right: Line profiles from B07. Line identifications are indicated on the plots. Several lines from the S11 data (middle) have ‘gaps’, thus the region marked in blue on the median, corresponding to these missing regions, should be deemed less reliable.

$K$-, $L$-, and $M$-band) in 3 epochs: 1986, 2001-2002, and 2011-2012. Each of the CO ro-vibrational datasets are all collected during or shortly after one of these epochs (S11 in 2001-2002, B07 in 2002, and B14 in 2012). Hence the observed variations of the CO ro-vibrational line profiles are not directly linked to the increased NIR brightness epochs. Meanwhile, this does not exclude that one underlying mechanism could in fact be driving both the NIR variability and the CO ro-vibrational variability in different ways.

From all three datasets we find broad emission lines (FWHM ~ 50-80 km/s) suggesting that the CO ro-vibrational lines are emitted from the inner radius of the disc. However, the FWHM measured from the three sets are not in agree-
4.3 Observational results

In Fig 4.1, we show the FWHM versus $J_{\text{up}}$ for lines collected from all three datasets. The FWHM variations can also be seen from the medians collected for high, mid and low $J$ separately, displayed in Fig 4.3 and listed with FWHM in Table 4.1. We see that lines from S11 are overall wider than those from B14. Low $J$ lines from B07 are narrower than both B14 and S11, but high $J$ lines from B07 are comparable in FWHM to S11. As discussed above, the B07 dataset has several irregular lines, which may be due to imperfect telluric corrections. Thus for the further comparison we focus on the B14 and S11 datasets.

From Table 4.1 we additionally see, that while the FWHM are not consistent between the datasets the FWZI (Full Width at Zero Intensity) for B14 and S11 are the same within error estimates. To explore this we also compare flux calibrated line profiles for individual transitions that were present in both S11 and B14 (Fig 4.4). This shows that the general width of these profiles are the same in the two datasets, while (in the case of high and medium $J$ lines) the intensity and the shape of the central part of the lines differ. For low $J$ (the P4 line) the shape is well matched in the two data sets. An interpretation could be that the single peaked line profiles (i.e. lines from the CRIRES data and low $J$ lines from the NIRSPEC data) are composites of multiple emitting regions, where the main (Keplerian) components are the same in the two epochs and the additional component, present in lines from B14 and in low $J$ lines from S11, could be related to the NIR variability. This additional component would then ‘drive’ the FWHM in B14 to lower values, since the half maxima location is shifted upwards.

The comparison of the flux calibrated lines should be considered with caution. Converting the continuum flux values from Jansky (S11, 12.1 Jy and B14, 16.3 Jy) to magnitudes, we find $M=2.85$ for S11, and $M=2.53$ for B14. The brightest state reported for HD 163296 is $M=2.90$ (de Winter et al. 2001). The magnitude derived from the S11 data is close to the brightest state, but the magnitude derived from the B14 data is $\sim0.4$ magnitudes brighter. In the $L$-band the amplitude of the variability does not exceed 0.2-0.3 magnitudes (Ellerbroek et al. 2014). Thus, a 0.4 magnitude increase in the $M$-band, compared to the brightest state (as inferred by our flux calibration) is unlikely. A more likely explanation would be that the error in the flux calibration of B14 is closer to 50%.

With the higher flux calibration uncertainty one could envision an alternative scenario for the line profile variability: If the continuum flux from the S11 data is instead stronger than those from B14 the central height of line from the two data sets might match, and the line wings would instead differ. Thus the line variability would be due to a broader wing component present in S11, in particular for high and medium $J$ lines. This would imply a single peaked main (constant) component and a variable broad (high velocity) component.
Figure 4.3 – Median line profile comparisons for the data from B14 (blue), S11 (red) and, B07 (black). Ranges of $J$-levels used for (co-addition) medians are indicated on the plots.

4.4 Model description

We use a previously published ProDiMo disc model for HD 163296 by Tilling et al. (2012). ProDiMo is a radiation thermo-chemical disc code (Woitke et al. 2009, Kamp et al. 2010), which solves the radiative transfer, the chemical network and the gas heating cooling balance. The Tilling et al. (2012) model assumes a parameterised disc structure using power laws for the surface density and the gas scale height. Level populations are calculated from statistical equilibrium and detailed line transfer calculations are performed to predict emission lines. In order to model CO ro-vibrational emission lines, we use the large CO ro-vibrational model described in Thiel et al. (2013). We include fluorescence pumping to the $A^1\Pi$ electronic level and use 40 rotational levels within 7 vibrational levels of both the ground electronic state $X^1\Sigma^+$ and the excited state $A^1\Pi$.

The Tilling et al. (2012) model has been computed using a Monte-Carlo evolutionary $\chi^2$-minimisation strategy (Woitke et al. 2011), varying 11 parameters to find the best fit to observed emission lines (not including the CO ro-vibrational lines) and the dust spectral energy distribution (SED), from HD 163296, simultaneously. The spatial CO emission maps were not used as a constraint for the modelling, however, the extracted line profiles for rotational CO lines (Isella et al.
Figure 4.4 – Individual line profile comparison of flux calibrated lines, that were present in both the B14 data (blue) and the S11 data (red). Line identifications are noted on the plots.

2007) were used as a constraint for the radial extent and tapered edge.

Key parameters used in the model are displayed in Table 4.2. The gas volume density profile, the gas temperature and the CO abundance are shown in Fig. 4.5. In Table 4.3 emission line predictions from the model are compared to the observed lines from literature. Even though this model has not been made to fit CO ro-vibrational observations, we use it here to investigate the emitting region of CO ro-vibrational transitions and to compare with observations.
Table 4.2 – Key model parameters and the assumed values (for more details see Tilling et al. 2012).

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>inner radius</td>
<td>R_{in}[au] 0.45</td>
</tr>
<tr>
<td>outer radius</td>
<td>R_{out}[au] 700.0</td>
</tr>
<tr>
<td>tapering-off radius</td>
<td>R_{taper}[au] 125.0</td>
</tr>
<tr>
<td>stellar luminosity</td>
<td>L_{*}/L_{\odot} 37.7</td>
</tr>
<tr>
<td>stellar mass</td>
<td>M_{*}/M_{\odot} 2.47</td>
</tr>
<tr>
<td>effective temperature</td>
<td>T_{eff}[K] 9250.0</td>
</tr>
<tr>
<td>disc mass</td>
<td>M_{disc}/M_{\odot} 0.071</td>
</tr>
<tr>
<td>dust to gas ratio</td>
<td>dust-to-gas 0.01</td>
</tr>
<tr>
<td>dust grain mass density</td>
<td>\rho_{\text{grain}}[g/cm^3] 3.36</td>
</tr>
<tr>
<td>minimum grain size</td>
<td>a_{\text{min}}[\mu m] 0.01</td>
</tr>
<tr>
<td>maximum grain size</td>
<td>a_{\text{max}}[\mu m] 2041</td>
</tr>
<tr>
<td>dust size dist. power index</td>
<td>P 3.68</td>
</tr>
<tr>
<td>flaring index</td>
<td>\beta 1.066</td>
</tr>
<tr>
<td>distance</td>
<td>dist [pc] 118.6</td>
</tr>
<tr>
<td>PAH abundance relative to ISM</td>
<td>f_{PAH} 0.0068</td>
</tr>
<tr>
<td>inclination</td>
<td>incl. 50.0°</td>
</tr>
</tbody>
</table>

Table 4.3 – Model CO line fluxes (from escape probability) compared to CO high J rotational lines observed with Herschel/PACS (Tilling et al. 2012), low J rotational lines observed from the ground (Isella et al. 2007), and ro-vibrational lines from S11.

<table>
<thead>
<tr>
<th>Mol.</th>
<th>\lambda [\mu m]</th>
<th>Obs. [10^{-18}W/m^2]</th>
<th>Model [10^{-18}W/m^2]</th>
</tr>
</thead>
<tbody>
<tr>
<td>^{13}\text{CO J}=1-0</td>
<td>2720.41</td>
<td>0.0124</td>
<td>0.0105</td>
</tr>
<tr>
<td>CO J=2-1</td>
<td>1300.4</td>
<td>0.379</td>
<td>0.40</td>
</tr>
<tr>
<td>CO J=3-2</td>
<td>866.96</td>
<td>1.65</td>
<td>1.21</td>
</tr>
<tr>
<td>CO J=18-17</td>
<td>144.78</td>
<td>&lt;13.1</td>
<td>2.69</td>
</tr>
<tr>
<td>CO J=29-28</td>
<td>90.16</td>
<td>&lt;11.1</td>
<td>0.624</td>
</tr>
<tr>
<td>CO v=1-0 P37</td>
<td>5.053</td>
<td>60.3</td>
<td>122.</td>
</tr>
<tr>
<td>CO v=1-0 P14</td>
<td>4.793</td>
<td>86.5</td>
<td>71.3</td>
</tr>
<tr>
<td>CO v=1-0 P4</td>
<td>4.700</td>
<td>158</td>
<td>70.8</td>
</tr>
</tbody>
</table>
Figure 4.5 – Left panel: Gas volume density, together with contours showing $A_V=1.0$ and $A_V=10.0$ (dashed white lines), $A_{V,rad}=0.1$, and $A_{V,rad}=1.0$ (dashed red lines). Middle panel: Gas temperature, together with contours showing $A_V=1.0$ and $A_V=10.0$ (white dashed lines), and gas temperature contours at 20, 40, 100, 300 and 1000 K (black dashed lines). Right panel: CO abundance, together with contours showing $A_V=1.0$ and $A_V=10.0$ (dashed white lines) and $\log(\chi/n)=-3$ (dashed blue lines).
Figure 4.6 – Line profiles from detailed line radiative transfer for the three lines v(1-0)P04, v(1-0)P14, and v(1-0)P37. The line wavelength, flux, FWHM and peak separation derived from the line profiles can be found on the plot. The thin black line represents the profile convolved with the NIRSPEC/Keck resolution (R=25000).
Figure 4.7 – Line and continuum optical depth, the cumulative line flux, and the CO density, as a function of radius, for the same three modelled lines. The line wavelengths and fluxes from simple vertical escape probability are indicated on the plot. Vertical dashed lines indicate the radii within which 15% and 85% of the total flux is emitted, the black box indicates the radial and vertical region from which 50% of the flux originates, and the red contour lines represent gas temperatures of 100 K and 300 K.
4.5 Model results

In Fig. 4.6 line profiles (calculated from detailed line radiative transfer) of three representative CO ro-vibrational emission lines, v(1-0)P04, v(1-0)P14, and v(1-0)P37, are shown together with line flux, FWHM and peak separation estimates derived from the line profiles. These three lines have similar shape, indicating that line shapes do not vary strongly with J. The peak separations in the modelled lines are $\sim$50 km/s, and the NIRSPEC resolution should thus be good enough to separate the peaks. In the upper panels of Fig 4.8 the peak separation, the FWHM, and the line fluxes are shown for selected line transitions (the observed line sample and a few extra lines to fill in gaps in J coverage) from the model. The lower panels show these same plots with all transitions calculated in LTE. For comparison we also show the observed peak separations, FWHM, and line flux. To obtain a more realistic comparison between model and observation, we add appropriate noise (S/N $\sim$100 on the continuum) and convolve the model line profiles with the spectral resolution of the instrument used for observations (CRIRES: 3 km/s, NIRSPEC: 12 km/s). Simulated CRIRES and NIRSPEC line profiles of three representative CO ro-vibrational transitions (v(1-0)P04, v(1-0)P14, and v(1-0)P37) are shown in Fig. 4.9.

The simulated CRIRES and NIRSPEC line profiles from the models have FWZI around 130-140 km/s. This is similar the observed FWZI (see Table 4.1). The FWHM values predicted by the model are in agreement with the FWHM for high J lines (and a few of the low J lines) from S11. The modelled mid J lines are too wide compared to observed mid J lines from S11 and all lines from B14 (Fig. 4.8). The line fluxes predicted by the model also match the observed high J line fluxes (S11 and B14) but the overall shape of the line flux versus J curve is different than what is observed.

The model predicts clear double peaks for all lines (significant central depression between peaks), which is not seen in the NIRSPEC observations. This could indicate that lines not only from B14 but also from S11 have a second non-Keplerian component, although much weaker in S11 than in B14. We do see indications of double peaks present in some observed lines (S11) and the peak separations measured from these are similar to the modelled lines (mostly high J transitions). However, the absence of a strong double peak could also be due to many lines in the S11 sample suffering from low transmission at the centre of the line, due to strong telluric absorption lines (see Sect. 4.3). The high J transitions are less likely to be significantly affected by telluric absorption and lend themselves better for a comparison to the models. In Fig. 4.10 we show flux normalised medians from the simulated CRIRES line profiles and NIRSPEC line profiles together with the corresponding observed (B14, S11) median line profiles. We show both medians made from all J transitions and medians made from only high or low J transitions.

\[\text{FWZI of the lines is determined by the inner radius of the disc. In the model the inner radius is set to 0.45 au, while values derived from observations lie in the range 0.2-0.55 au (Renard et al. 2010, Eisner et al. 2009, Tannirkulam et al. 2008, Benisty et al. 2010).}\]
lines in the sample. We can confirm that the high $J$ median from the S11 sample does in fact compare well to the model. Looking in particular at the line wings, the median from all lines and the median from high $J$ lines from S11 match well. The match with the line wings of the medians from B14 and the low $J$ median from S11 is not good. In these cases, the line profiles might be multiple component profiles with a non-Keplerian, central component. Thus, the direct comparison of these lines with the models can be misleading, since the model contains only a disc component. We can obtain a match between the line wings of the observed B14 lines and the simulated CRIRES line profiles by re-normalising the median line profile to the wings of the model (multiplying the normalised CRIRES median by 1.9). A similar match could also be achieved for the low $J$ median from S11 (multiplying the normalised median by 1.4). Thus, assuming the presence of an extra component, the model line wings match the observations very well given the S/N of the data.

The shape of a line profile is determined by how the flux builds up as a function of radius. In Fig. 4.7 we show a radial profile of the cumulative line flux from the model. From the peak separation of the high $J$ lines from S11, we infer an outer radius for the emitting region of $\sim 2.1 \pm 2.0$ au, using the assumption of Keplerian rotation. In the model, 85% of the emission builds up within 1.5 au. Thus, the model provides a good prediction of the emitting region. In summary, provided there is a non-Keplerian additional component in the lines from B14 and in the low $J$ lines from S11, the model fits the observed CO ro-vibrational lines of HD 163296 overall very well.
Figure 4.8 – Upper panels: The peak separations (left), the FWHM (middle), and the line fluxes (right), as a function of $J_{up}$ for the modelled sample of CO fundamental ro-vibrational (black squares). The green squares are the model convolved with the NIRSPEC resolution (the model convolved with the CRIRES resolution corresponds very closely to the un-convolved model and is therefore not shown). Observations are shown for comparison as blue crosses (CRIRES, B14) and red crosses (NIRSPEC, S11). In addition to the displayed error bars for the observed lines, there is also an additional systematic error of 50% for the B14 data and 20% for the S11 data. This error has a similar effect on all lines, and thus do not affect line ratios. Bottom panels: The same plots with the lines calculated in LTE.
Figure 4.9 – Simulated observed line profiles for three modelled lines. From left to right: v(1-0)P04, v(1-0)P14, and v(1-0)P37. The line profiles are convolved with the CRIRES resolution (R=100 000) (top panels) or the NIRSPEC resolution (R=25 000) (lower panels) and a signal to noise ratio of 100 on the continuum is applied. The line wavelength, flux, FWHM and peak separation of the (un-convolved) model are reported on the plot, and the thin red line is that of the un-convolved profile without noise.
4.6 Boltzmann diagrams

Boltzmann diagrams with the line fluxes from an observed sample of lines are often used to estimate the CO column density and the rotational temperature. In B14 these kind of Boltzmann diagrams were created for an observed sample of discs, including HD 163296. Details about the construction of these Boltzmann diagrams can be found in B14 and van der Plas et al. (2014).

In B14 we pointed out that a better $J$ coverage was necessary in order to get more precise and reliable rotational temperatures. We also noted that higher $J$ levels than those observed ($40 < J < 60$) might be needed in order to derive rotational temperatures from optically thin lines that correspond to the physical gas temperature in the emitting regions of these transitions (Thi et al. 2013). Using the line fluxes from both observations (B14) and from the ProDiMo model (calculated from simple vertical escape probability$^3$), we now have the opportunity to test these issues with the disc model. In Fig. 4.11 we compiled a selection of Boltzmann diagrams with differing line samples: a) A Boltzmann diagram compiled from the observed line fluxes from B14 (the line sample used is that seen in the left panel of Fig 4.2). b) A Boltzmann diagram compiled from the modelled line fluxes where a full $J$ coverage, from $J=0$ to $J=40$, is used. c) A Boltzmann diagram compiled from the modelled line fluxes where no high $J$ lines are used ($J<20$). d) A Boltzmann diagram compiled from the modelled line fluxes where no low $J$ lines are used ($J>10$). e) A Boltzmann diagram compiled from the modelled line fluxes where the sample of lines used is identical to the observations from B14. f) A Boltzmann diagram compiled from the modelled line fluxes calculated in LTE with a line sample identical to the observations from B14.

For all the presented Boltzmann diagrams we also provide best fit contour plots with 1-, 2-, and 3$\sigma$ confidence intervals for the fitted temperatures and CO column densities (Fig. 4.12). For the modelled line fluxes, a 10% error is assumed. These plots reveal that the derived temperatures are highly degenerate, and in most cases all temperatures in the fitting range give a reasonable fit to the data. Smaller error bars can give better constraints, but observations seldom offer high accuracies on continuum placement, that would reasonably allow such smaller error bars. Furthermore, this type of simple slab model can never reach a solution with wave patterns that the data here displays, leading to degeneracies in the fitted values, since no ‘perfect’ match can be found.

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$^3$ Differences between fluxes calculated from escape probability and detailed line radiative transfer typically amount to <20%. For examples see Figures 4.6 4.7.
Figure 4.10 – Upper panels: Medians of the normalised modelled line profiles (green line) with the individual modelled line profiles (dotted black lines) with an applied signal to noise ratio of 100 and the spectral resolution of CRIRES (left) or NIRSPEC (right). For comparison, the observed line profile median is overplotted (B14, dashed blue line and S11, dashed red line). Medians created using only the low $J$ lines ($J<10$) shown in the middle panels, and medians created using only the high $J$ lines ($J>20$) shown in the lower panels. For the CRIRES medians and the low $J$ NIRSPEC median, we additionally overplot the observed medians normalised to the line wings of the model median to evaluate the presence of an additional non-Keplerian component.
Figure 4.11 – Boltzmann plots for CO ro-vibrational ν=1-0 transitions from model and observations of HD 163296. The black symbols are the input lines, and the best fit for the rotational temperature, $T_{\text{rot}}$, is shown by red lines (upper line: P branch, lower: R branch). The Boltzmann model predictions for input lines are shown as red squares, and the grey areas around the best fit lines are the 1σ areas shown in Fig. 4.12. The model predictions for $T_{\text{rot}}$ and $N_{\text{CO}}$ are printed on the plots. From the top left: a) A diagram compiled from the observed line fluxes (B14). b) A diagram from a full $J$ coverage sample (0<$J<$40) of modelled line fluxes. c) A diagram from modelled line fluxes where no high $J$ lines are used ($J<$20). d) A diagram from modelled lines where no low $J$ lines are used ($J>$10). e) A diagram from modelled lines where the sample of lines used is identical to the observed sample from B14. f) A diagram from modelled lines (observed sample, B14) with the lines calculated in LTE.
Figure 4.12 – Best fit contours for the Boltzmann diagrams (Fig. 4.11), displaying the 1 $\sigma$ (green), 2 $\sigma$ (yellow), 3 $\sigma$ (orange), and >3 $\sigma$ (red) confidence intervals of the fitted temperature and CO column density.
Chapter 4 – CO ro-vibrational lines from HD 163296

The rotational temperature derived from the observations is, within the error estimates consistent with all the modelled rotational temperatures. However, the degeneracy is very large, since uncertainty estimates for the observed line fluxes are as large as 15-35%.

We extract from the disc model the average gas temperature in the line emitting volume (estimated from escape probability) for each CO ro-vibrational line using

\[
\langle T_{\text{gas}}(\text{line}) \rangle = \frac{\int_{V_{15}}^{V_{85}} T_{\text{gas}}(r, z) n_{\text{CO}}(r, z) \, dV}{\int_{V_{15}}^{V_{85}} n_{\text{CO}}(r, z) \, dV} .
\] (4.1)

Here the volume boundaries \( V_{15} \) and \( V_{85} \) are outlined by the radii \( r_{15} \) and \( r_{85} \) and the heights \( z_{15} \) and \( z_{85} \) within which 15 \% and 85 \% of the flux originate radially and vertically. The derived average gas temperature of the various transitions are all very similar with an average temperature of \( 657^{+33}_{-7} \) K (Fig. 4.13). The Boltzmann diagrams using a full \( J \) coverage of modelled line fluxes yields a rotational temperature \( (T_{\text{rot}}=625 \text{ K}) \) which is only 32 K lower than the average gas temperature. However, the wave pattern at high \( J \) transitions (near \( E_{\text{up}} \sim 6000 \text{ K} \)) is not well fitted. The rotational temperatures derived from modelled line fluxes excluding either high \( J \) lines or low \( J \) lines are respectively 75 K and 25 K higher than the rotational temperature from the full coverage diagram. The comparison of \( T_{\text{rot}} \) from these two diagrams, to the average gas temperature is as good as from the full coverage diagram. The ‘no high \( J \)’ diagram is 43 K too high, and the ‘no low \( J \)’ diagram is only 7 K below \( (T_{\text{rot}}=700 \text{ K and } T_{\text{rot}}=650 \text{ K, respectively}) \). Thus,

\[ \text{Figure 4.13} \] – Physical gas temperatures in the emitting region of the individual lines in the model as a function of \( J \) level.
with dense \( J \) coverage one could estimate the gas temperature in this disc from a derived rotational temperature, even when excluding either the higher or lower \( J \) transitions from the calculations.

The rotational temperature \( T_{\text{rot}} = 425 \text{ K} \) derived from the Boltzmann diagram, using modelled line fluxes and the observed sample of lines, is 232 K too low compared to the average gas temperature. This could relate to the fact that, by chance, the observed sample covers just a few of the high \( J \) levels at the maximum of the wave pattern (\( E_{J_{\text{up}}} \sim 6000 \text{ K} \)) in the Boltzmann diagram, and in this way drives the fit to a very different temperature. Thus, a sparse line sample spread out over the full \( J \) range does not yield as good a temperature estimate as a full sample over a limited \( J \) range.

The modelled line fluxes used in these presented Boltzmann diagrams have been calculated including both IR and UV pumping in addition to collisional excitation, whereas the Boltzmann diagrams have been made using a single temperature slab model only taking into account LTE conditions. Thus, for comparison we also present a Boltzmann diagram (using the observed sample of lines) with modelled lines calculated in LTE (a direct line flux comparison between the modelled line fluxes and the LTE modelled line fluxes can be made by comparing upper and lower left panels of Fig. 4.8). This diagram shows a much steeper and straight slope (no wave pattern) and the best fit results in \( T_{\text{rot}} = 825 \text{ K} \). In this case the fit yields much better constraints on the derived rotational temperatures (less degeneracy, Fig. 4.12). However, the lines calculated in LTE have narrower peak separation compared to the non-LTE lines, indicating a much larger outer radius for the emitting region, while the inner radius given by the FWZI stays the same. This will lower the average gas temperature derived in the CO emitting region compared to the non-LTE values. Since the line emitting region now stretches over a large radial range, a single slab model with a fixed density and temperature cannot describe the conditions under which the LTE lines originate.

4.7 Discussion

4.7.1 Observed line profile comparison

B14 and S11 show clear differences in the line profile shapes that instrumental differences alone cannot explain. The single peaked nature of the B14 lines points at variability in the lines as an explanation. Furthermore, the model predicts double peaked line profiles which only match the line profiles collected by S11 for high \( J \). A possible explanation could be that an additional non-Keplerian CO ro-vibrational emission component is present in both S11 and B14, but that this component is weaker in S11.

Comparing line fluxes, the overall shape or curvature in line flux versus \( J \) diagram agrees well between S11 and B14, and the line flux values are also similar. Hence, the line fluxes alone do not indicate any kind of variability in the lines.
However, the flux calibration, is rather uncertain, around 50% for B14 and 20% for S11, and thus the similarity in line fluxes does not necessarily exclude variability.

### 4.7.2 Model comparison

The overall agreement between the model and the observations is good, considering the fact that it was not set up to fit these lines initially. The peak separation and the FWHM matches the values from S11 at high $J$. If all other lines are affected by the presence of an additional non-Keplerian component (that is not included in the model), the FWHM or peak separation of the observed lines cannot be expected to match the Keplerian lines of the model.

The individual line fluxes predicted by the model are all within a factor of two of the observed values. In particular, low and mid $J$ are typically a factor two too low compared to observations, while the modelled high $J$ lines match the observed line fluxes better. The overall shape of the flux versus $J$ diagram is not well fitted by the model. The modelled lines calculated in LTE give a much better shape prediction for the flux versus $J$ diagram, but the line fluxes are in this case almost a factor of ten too high. This is a difference that cannot be explained by flux calibration uncertainties (B14, 50% systematic flux calibration uncertainty, S11, 20% systematic flux calibration uncertainty).

A possible explanation for the difference in flux versus $J$ curvature between model and observations, could be additional flux contributed by a non-Keplerian component with different strength at high and low $J$. Subtracting the Keplerian component predicted by the model from the observed line profiles normalised to the line wings (see Fig. 4.14), we infer a non-Keplerian component that contributes 39% of the line flux in the high $J$ median from B14, and 57% of the line flux in the low $J$ median from B14. For the S11 data we find no clear detection of the non-Keplerian component in the high $J$ median, and we infer a 23% contribution to the line flux in the low $J$ median. In all detected cases, the inferred non-Keplerian component is centred on the Keplerian component, and present at velocities ranging from -20 km/s to +20 km/s. The agreement of the velocities in the inferred non-Keplerian components, supports this hypothesis. Subtracting the above estimated line flux contributions of the non-Keplerian component from the total observed line fluxes does shift the observed line fluxes in the right direction with respect to the modelled values, and the overall shape of the flux versus $J$ diagram is somewhat flatter (Fig. 4.15).

### 4.7.3 Variability of the CO ro-vibrational lines

The variability of HD 163296 is documented in the literature (Sitko et al. 2008, Ellerbroek et al. 2014). Ellerbroek et al. (2014) suggest a scenario where dust clouds are launched above the disc plane and cross the observers line of sight.
Klaassen et al. (2013) detected a rotating molecular disc wind from HD 163296 using ALMA. The authors interpret this as a low velocity wind (<25 km/s) launched at a few au. This wind could be the cause of the non-Keplerian component that we detect (velocities ±20 km/s). A low velocity molecular outflow containing CO, could be emitting CO ro-vibrational lines as it is launched above the usual disc emitting region. Instabilities in the inner disc could lead to episodic disc winds of varying strength resulting in e.g. stronger non-Keplerian components present in the B14 data compared to the S11 data. Fig. 4.16 shows a schematic view of the combined geometry of the disc, the wind and the CO ro-vibrational emission. Pontoppidan et al. (2011) showed with their wind model that if the line of

Figure 4.14 – Medians of the normalised modelled line profiles (green lines), the observed line profiles normalised to the maximum and to the line wings of the model (B14, dashed blue lines and S11, dashed red lines), and the observed (line wing normalised) median minus the modelled median (black lines). The medians in the upper panels are created using only the low \( J \) lines \((J<10)\), and medians in the lower panels are created using only the high \( J \) lines \((J>20)\).
Figure 4.15 – Pure Keplerian line fluxes from B14 (blue) and S11 (red), based on the estimates of the non-Keplerian components. The modelled line fluxes are included (black squares). In addition to the displayed error bars for the observed lines, there is also an additional systematic error of 50% for the B14 data and 20% for the S11 data. This error must have a similar effect on all lines, and can not act to change the line ratios.

sight falls close to the angle of the wind column, self-absorption can occur in the line profile. The fact that no CO ro-vibrational self-absorption is detected in lines from either B14 or S11, puts strong constraints on the wind model. With the disc inclination of 50° the wind column has to be launched at minimum 60°-70° (with respect to the disc plane), almost vertically from the disc. If the wind column is at lower inclinations, crossing the line of sight of the observer, the CO gas has to have either no sharp temperature gradient (colder gas would cause absorption), or the CO would have to dissociate before it can significantly cool.

New observations of the CO ro-vibrational lines collected with either NIRSPEC/Keck or CRIRES/VLT are necessary to both exclude all instrumental differences and add additional epochs for future line profile comparison studies. Given the difficulties with the near-IR observational window, observations of Neon fine structure lines ([Ne ii] at 12.81 µm and [Ne iii] at 15.55 µm) could be an alternative. Baldovin-Saavedra et al. (2012) detected and spectrally resolved the Ne ii in seven stars using VLT/VISIR, where one was the first detection of Ne ii from a Herbig Ae/Be star (V892 Tau). The Ne ii lines are complementary to the CO ro-vibrational lines since they probe vertical heights above the molecular layer over a range of radial distances (out to 10-15 au, Glassgold et al. 2007). Hence, if a molecular outflow is causing variable non-Keplerian CO ro-vibrational emission components, the variability could also be detectable in the [Ne ii] line.

An alternative scenario to the non-Keplerian central component caused by a
4.7 Discussion

disc wind, is one where the line shape differences are due to additional line wings present in the S11 data. This could be due to an additional broad double peak component caused by episodic accretion onto the disc (seen in the case of T Tauri stars). The enhanced accretion creates funnel flows seen as broad double peaked lines (Najita et al. 2003). Variable accretion has in fact been noted by Mendigutía et al. (2013) for HD 163296. From their comparison with previous results they found that the accretion rate of HD 163296 is more or less constant on timescales of days to months. However, the accretion rate derived using data from 2011-2012, was found to have increased by more than 1 dex over a timespan of 15 years. Thus the B14 dataset was collected during a high accretion rate period, and should thereby be displaying this additional line wing component. Yet, opposite to what we would expect from the high accretion rate, the lines from the B14 data (2012) are narrower than lines from the earlier epoch (S11, 2002). Hence, an additional line component due to episodic accretion does not offer an explanation to the observed line variability.

![Figure 4.16](image)

**Figure 4.16** – Sketch of the geometry of HD 163296 and the disc wind and how this could relate to the variability of the CO ro-vibrational lines (Inspired by Ellerbroek et al. 2014). The blue areas indicate the possible CO ro-vibrational emission regions. The hatched blue area indicates CO ro-vibrational emission from the wind just above the disc.

4.7.4 Rotational temperatures versus physical gas temperatures

From a series of tests with Boltzmann diagrams we see that in most cases, the derived rotational temperatures are highly degenerate. This is due to the limita-
tions of the simplified single temperature LTE slab model used to fit the data. The wave pattern that we see in the Boltzmann diagrams from the thermo-chemical disc model cannot be reproduced by a simple slab model. These wave patterns were earlier seen in the Boltzmann diagrams constructed by Thi et al. (2013), for a generic Herbig thermo-chemical disc model even in cases where the UV-pumping was switched off. Only discs with gaps (or optically thin lines) showed a much flatter curve, and can thus be well fitted by a simple slab model. This is confirmed in the disc around HD 100546, which hosts a gap out to $\sim 10$ au, and shows a flat Boltzmann diagram with only a curve up at low energies (no wave pattern) (Hein Bertelsen et al. 2014, Chapter 2).

However, if we disregard for a moment the large degeneracies, a scattered sample of $J$ transitions, with smaller ‘gaps’ in the coverage (such as the observed samples of lines), does not lead to a good estimate of the true gas temperature in the line emitting region of this disc. Such a selection also fails in estimating the rotational temperature of a full $J$ coverage diagram. A diagram with dense coverage over a restricted $J$ range, such as the lack of either high or low $J$ lines gives a rotational temperature closer to the full sample diagram value and to the true gas temperature of the line emitting region in the model. The high degeneracies for the derived temperatures mean that we cannot confirm whether similarities between $T_{\text{rot}}$ and $T_{\text{gas}}$ (in the cases of the full $J$ coverage diagram or the dense coverage restricted $J$ range diagrams), are merely a coincidence occurring in this disc. More tests using a series of disc models are needed to investigate this further.

We emphasise that the best way to use the rotational temperatures derived from these Boltzmann diagrams is in a comparative manner: When different discs are compared to one another or models are compared to observations and line samples have similar $J$ coverage. Additionally, discs with gaps might yield more meaningful gas temperature estimates, since their slopes tend to be better reproduced by simple slab models.

4.8 Conclusions

We have compared CO ro-vibrational lines from high-resolution NIR spectra for HD 163296, collected at different epochs (2002,2012) with different instruments (NIRSPEC/Keck, CRIRES/VLT), separated by $\sim 10$ years. We find significant differences in line shapes. In particular, double peaks are only present in one epoch, and mainly in high $J$ transitions. FWHM measurements are significantly wider in the 2002 epoch. The FWZI of all profiles is, however, similar. Comparison of flux calibrated lines indicates that line wings could be similar at the two epochs and an additional component at lower velocities likely causes the FWHM difference and the peak differences. However, the reliability of the flux calibration is limited (errors of $\sim 50\%$ for B14 and $\sim 20\%$ for S11).

We also present modelled CO ro-vibrational emission lines produced using a previously constructed ProDiMo model (Tilling et al. 2012), that was fitted to
observed emission lines (not including the CO ro-vibrational lines) and the dust spectral energy distribution (SED) from HD 163296. The model predicts the peak separation, the FWHM, and the line flux of the high $J$ lines from S11 well. For all observed lines from B14 and the lower $J$ lines from S11, the peak separation is not seen (single peaks or ambiguous flat tops), the FWHM are a factor 1.6 higher than in B14 and a factor 1.1 higher than in S11, and the line flux of the model is up to a factor three too low compared to observations.

We propose that an additional non-Keplerian component of the CO ro-vibrational emission is present in the B14 data set. In the epoch of the S11 lines, the non-Keplerian component is also present, but significantly weaker. The line flux contribution of the proposed non-Keplerian component decreases with $J$ for both data sets, and is thus only detectable for low $J$ lines in the S11 data set. Subtracting the modelled double peaked medians from the observed high and low $J$ medians, for both epochs separately, we find a non-Keplerian component from the observed lines, present at similar velocities in all cases (and not detectable at high $J$ in S11). This would explain why the model underestimates line fluxes, FWHM, and peak separation, for low and middle $J$ lines. We suggest that this non-Keplerian component could be due to the molecular disc wind detected by Klaassen et al. (2013). Further observations are necessary to confirm the nature of the variability seen for these lines (with CRIRES/VLT or NIRSPEC/Keck) and the presence of a variable disc wind component. The latter could be done with or VISIR/VLT observations of the [Ne II] line.

Lastly, we presented a comparison between Boltzmann diagrams compiled from CO ro-vibrational lines from a ProDiMo model of HD 163296, using varying line sampling, and a diagram compiled from the observed CO ro-vibrational lines from HD 163296 (B14). We find a high level of degeneracy in the fitted temperatures and can thus not draw any strong conclusions based on the comparison between modelled and observed lines. The degeneracy of the temperatures is due to the poor fit of the single temperature slab model to the typical wave pattern that is present in the Boltzmann diagrams compiled from line fluxes of thermo-chemical disc models. Diagrams from discs hosting gaps (or when lines are optically thin) show much straighter slopes (e.g. HD 100546, Hein Bertelsen et al 2014), and the single temperature slab model presents a better fit. We suggest that Boltzmann diagrams, produced with sparse $J$ sampling, should only be used for comparison purposes, i.e. comparing observations with the same $J$ coverage or comparing observations with detailed disc models.

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