PROBING THE RADIAL TEMPERATURE STRUCTURE OF PROTOPLANETARY DISKS WITH HERSCHEL/HIFI

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ABSTRACT

\textit{Herschel/HIFI} spectroscopic observations of CO $J = 10$–$9$, CO $J = 16$–$15$ and [C ii] toward HD 100546 are presented. The objective is to resolve the velocity profile of the lines to address the emitting region of the transitions and directly probe the distribution of warm gas in the disk. The spectra reveal double-peaked CO line profiles centered on the systemic velocity, consistent with a disk origin. The $J = 16$–$15$ line profile is broader than that of the $J = 10$–$9$ line, which in turn is broader than those of lower-$J$ transitions ($6$–$5$, $3$–$2$, observed with APEX), thus showing a clear temperature gradient of the gas with radius. A power-law flat disk model is used to fit the CO line profiles and the CO rotational ladder simultaneously, yielding a temperature of $T_0 = 1100 \pm 350$ K (at $r_0 = 13$ AU) and an index of $q = 0.85 \pm 0.1$ for the temperature radial gradient. This indicates that the gas has a steeper radial temperature gradient than the dust ($\mean{\delta q_{\mathrm{dust}} \approx 0.5}$), providing further proof of the thermal decoupling of gas and dust at the disk heights where the CO lines form. The [C ii] line profile shows a strong single-peaked profile red-shifted by 0.5 km s$^{-1}$ compared to the systemic velocity. We conclude that the bulk of the [C ii] emission has a non-disk origin (e.g., remnant envelope or diffuse cloud).

\textit{Key word:} protoplanetary disks

\textit{Online-only material:} color figures

1. INTRODUCTION

The temperature distribution of the gas in protoplanetary disks is a fundamental ingredient in models of gas and dust dynamics and the processes which ultimately control disk evaporation and planet formation. Thermochemical models of disks show that the gas temperature is significantly higher than that of the dust in the upper layers of the disk, first investigated by Kamp & Dulcombe (2004) and Jonkeheid et al. (2004) and subsequently by many other groups (e.g., Glassgold et al. 2004; Gorti & Hollenbach 2004; Nomura & Millar 2005; Aikawa & Nomura 2006; Jonkeheid et al. 2006, 2007; Gorti & Hollenbach 2008; Ercolano et al. 2009; Woods & Willacy 2009; Woitke et al. 2009; Kamp et al. 2010). These layers also play a key role in the chemical evolution of the disk by forming molecules through high temperature gas-phase reactions (e.g., Aikawa et al. 2002; Woitke et al. 2010). However, the gas temperature in these layers is notoriously difficult to compute and existing models show large differences as reported by Röllig et al. (2007) for the case of photodissociation region models. Disk models span a wider range in gas density and irradiation conditions, with even larger associated uncertainties (see discussion in Visser et al. 2012). Addressing the physical properties of the gas in these layers directly through observations is thus important to test the various thermochemical disk models, which, in turn, provide the basis for the analysis of many other data.

Various observational studies have found evidence for vertical temperature gradients in the gas. The outer disk (>100 AU) has been probed by single dish (van Zadelhoff et al. 2001) and interferometric data (Dartois et al. 2003; Piétu et al. 2007) of various CO low-lying pure rotational lines. For the inner disk (<50 AU), evidence for a warm gas layer with $T_{\text{gas}} > T_{\text{dust}}$ was found by Goto et al. (2012) using spectrally and spatially resolved observations of CO ro-vibrational lines. At intermediate radii, the warm layers emit primarily at far-infrared wavelengths. Recent observations with \textit{Herschel}/PACS report the detections of pure rotational high-$J$ ($J_u > 12$, $E_u \geq 400$ K) CO emission lines in several protoplanetary disks (e.g., Sturm et al. 2010; van Kempen et al. 2010; Meeus et al. 2012, 2013). Modeling of the entire CO ladder for one source, HD 100546, clearly demonstrates the need for gas–dust decoupling in the upper layers throughout most of the disk (Bruderer et al. 2012). However, these spatially unresolved PACS data do not directly probe the radial location of the warm gas. We present here spectrally resolved \textit{Herschel}/HIFI data that uniquely determine the emitting regions through Kepler’s laws.

At a distance of 97 pc (±4 pc; van Leeuwen 2007), the Herbig Ae star HD 100546 is one of the best studied protoplanetary disks. Bruderer et al. (2012) presented a detailed analysis of the observed CO/CI/CII emission in this source. An unexpected conclusion was that the gaseous carbon abundance in this disk must be ~5 times lower than that in the interstellar medium (ISM). Their model, however, could not reproduce the strong [C II] emission detected with PACS, even after subtraction of the extended [C II] component (Sturm et al. 2010; Fedele et al. 2013). One possibility is that the [C II] flux measured with PACS is contaminated by a compact diffuse component, which can also be tested with spectrally resolved data.

This paper presents new \textit{Herschel}/HIFI observations of CO $J = 10$–$9$, $J = 16$–$15$ and [C II] toward the Herbig Ae star HD 100546. These spectra are compared to existing APEX sub-millimeter observations of lower-$J$ CO lines (6–5, 3–2,
Panić et al. 2010) with the aim of constraining the radial temperature, column density and emitting regions of warm CO and [C II] in the disk and to test the predictions of thermochemical models. Given the spread of upper level energy of the four CO lines of more than one order of magnitude, with $E_J = 33$ K and $E_J = 751$ K, a large range of temperatures can be probed.

2. OBSERVATIONS AND DATA REDUCTION

The CO $J = 16–15$ (ObsID: 1342247519), CO $J = 10–9$ (1342235779) and [C II] (1342247518) observations were executed in dual beam switch fast chopping mode with the Wide-Band Spectrometer (WBS) and the High Resolution Spectrometer (HRS) of the Heterodyne Instrument for the Far-Infrared (HIFI) simultaneously. The spectral resolution was set to 1.1 MHz for WBS and 0.25 MHz for HRS for both polarizations. Because of the diffuse [C II] emission, seen previously with PACS, the [C II] observation of has been carried out in “load chop” where an internal calibration source is used in combination with an “off-source” calibration observation. The half-power-beam-width (HPBW) is 18′′ at the frequency of the CO $J = 10–9$ line and 11′′ at the frequencies of the CO $J = 16–15$ and [C II] lines (Roelfsema et al. 2012), thus the beam encompasses the entire disk.

The spectra have been extracted from the level 2 data which have been processed with standard pipeline SPG v9.1.0. Standing waves are present in the WBS and HRS band 7 spectra of the CO $J = 16–15$ and [C II] lines. These have been removed by fitting a set of sine functions after masking the narrow spectral features (CO or [C II]). This operation was performed with the “fitHiFrFringe” script provided with Hipe. No significant differences are observed in the two polarizations and the final spectra are obtained by averaging the two polarizations (for WBS and HRS separately). The data are converted from antenna temperature to mean-beam temperature ($T_{mb}$) dividing by $\eta_A/\eta_l$, where $\eta_A$ is the beam efficiency (0.56 for CO $J = 10–9$ and 0.62 for CO $J = 16–15$ and [C II], respectively) and $\eta_l$ is the forward efficiency, 0.96 (Roelfsema et al. 2012). The spectra are shown in Figure 1.

3. RESULTS

The CO $J = 16–15$, CO $J = 10–9$ and [C II] lines are detected in the WBS spectrum. The [C II] line is also detected in the HRS spectrum.

3.1. CO

The HIFI/WBS spectra of the CO lines are shown in Figure 1 (top two panels), normalized to their peak intensity. The profiles of both lines show a characteristic double-peak profile created by the Keplerian motion of the gas in the protoplanetary disk around HD 100546. The lines are centered at $V_{LSR} = 5.6$ km s$^{-1}$ in good agreement with the system velocity measured using low-$J$ CO lines in the sub-millimeter (e.g., Panić et al. 2010). The $J = 16–15$ line is clearly broader than the $J = 10–9$ line. The integrated intensities and fluxes are reported in Table 1. The flux of the CO $J = 16–15$ line agrees well with the Herschel/PACS measurement (5.88 $\pm$ 0.97 $10^{-17}$ W m$^{-2}$; Meeus et al. 2013). The third panel of Figure 1 shows the $J = 3–2$ sub-millimeter line, which is narrower than both higher-$J$ lines with a velocity width of only $\Delta v_{peak} = 2.4$ km s$^{-1}$ ($\Delta v_{peak}$ refers to the peak-to-peak separation). Table 1 summarizes the observed widths with the maximum velocity broadening observed in the $J = 16–15$ line ($\Delta v = 5.3$ km s$^{-1}$). Because of high disk inclination (42°), the Keplerian motion dominates the line width, meaning that the narrow lowest-$J$ line traces the slowly rotating gas in the outer part of the disk and the wider highest-$J$ line traces faster gas located closer to the star.

\footnotesize

\textsuperscript{6} To convert the integrated intensity ($\int T_{mb} dV$, K m s$^{-1}$) to integrated flux ($W$ m$^{-2}$), the conversion formula is $2k \nu(e/c)^3\pi(HPBW/2\sqrt{\pi})^2 \int T_{mb} dV$, with $k$ (Boltzmann constant) in unit of W s K$^{-1}$, $\nu$ in Hz, $c$ in m s$^{-1}$, $T_{mb}$ in K.

\normalsize

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure1.png}
\caption{Herschel/HIFI spectra of CO $J = 16–15$, $J = 10–9$ and [C II] toward HD 100546, together with the APEX $J = 3–2$ spectrum (from Panić et al. 2010). The vertical dashed line shows the system velocity. The (blue) solid line is the best-fit power-law model (Section 4) and the (red) dashed is the prediction of the thermochemical model from Bruderer et al. (2012). (A color version of this figure is available in the online journal.)}
\end{figure}
3.2. [C II]

The [C II] spectrum is shown in Figure 1 with a spectral resolution of 1.1 MHz (0.17 km s\(^{-1}\)). At this resolution the line does not reveal a double-peaked profile characteristic of Keplerian motion. Moreover, because the line is centered ~0.5 km s\(^{-1}\) redward of the known system velocity, it is very likely that most of the [C II] line does not come from the disk.

4. ANALYSIS

The simplest possible model to analyze both the velocity profiles as well as the line intensities is a geometrically thin disk model in which temperature and column density are power-law functions of radius. The CO velocity profiles then constrain the radial temperature gradient of the gas while the line fluxes provide further constraints to the radial distribution of the gas column density. Specifically,

\[
N(r) = N_0 \left( \frac{r}{r_0} \right)^{-p} \quad T(r) = T_0 \left( \frac{r}{r_0} \right)^{-q},
\]

where \(r_0\) is the inner radius of the disk, 13 AU as found by van der Plas et al. (2009), and \(N_0, T_0\) are the column density and temperature at \(r_0\). The motivation to use a geometrically thin disk is the fact that the full thermochemical models (e.g., Bruderer et al. 2012) show that the high values of the line critical density, this assumption holds for all the CO lines analyzed here, Bruderer et al. 2012; the intrinsic line shape is Gaussian and the intrinsic width at each position is given by the thermal broadening plus turbulent broadening (fixed to \(v_{\text{turb}} = 0.3\) km s\(^{-1}\)).

4.1. Line Flux from a Rotating Disk

The line flux from a rotating disk is given by the integral over the disk surface

\[
F_v = \frac{\cos(i)}{d^2} \int_{r_0}^{1000} \int_0^{2\pi} B_\nu(T(r))(1 - e^{-\tau(r,\theta)})d\theta dr,
\]

which is defined by polar coordinates \((r, \theta)\). The line opacity is

\[
\tau(r, \theta) = \frac{\tau(r) \nu_{\text{proj}}(r, \theta)\cos(i)}{\nu}.
\]

with \(i (42^\circ)\) the disk inclination \((i = 0^\circ\) is edge on), \(d\) the distance, \(B_\nu(T)\) the Planck function and \(\tau(r)\) the opacity perpendicular to the disk surface. For a Keplerian rotating disk around a star with mass \(M_* (2.5\ M_\odot)\), the projected velocity is

\[
u_{\text{proj}}(r, \theta) = \sqrt{\frac{GM_*}{r}} \sin(i) \cos(\theta).
\]

The opacity of a line connecting two CO levels \(u\) and \(i\) is given by

\[
\tau_u = \frac{A_{ul}c^2}{8\pi\nu_u^2} N(r) \left( \frac{g_u}{g_i} - 1 \right) \times \frac{1}{\sqrt{\pi} \Delta \nu} e^{-\left( \frac{\nu}{\Delta \nu} \right)^2},
\]

where \(A_{ul}\) is the Einstein-A coefficient, \(x_i, u\) the normalized level population, \(g_i, u\) the statistical weights and \(\Delta \nu\) the intrinsic line width (Doppler-parameter). The molecular data are from Schöier et al. (2005). Assuming local thermodynamic equilibrium, the level population is given by \(x_i = g_i \exp(-E_i/kT)/Q(T)\), with the level energy \(E_i\) and the partition function \(Q(T)\). The telescope beam is represented by a Gaussian. The intrinsic line width contains contributions from turbulent and thermal broadening. The model profiles of the three lines are shown in Figure 1.

4.2. CO Velocity Profiles and Rotational Ladder

The fit of the CO ladder by itself is degenerate as different power-law indices are able to reproduce the line fluxes. The resolved profiles of the CO lines are needed to break this degeneracy. The best-fit parameters are found by minimizing the \(\chi^2\) (sum of the five individual \(\chi^2\); four for the velocity profiles and one for the line fluxes from the CO rotational ladder). The \(\chi^2\) minimization is performed in two steps: first a sparse grid of 10,000 models was created for 10 different values of the parameters in the following ranges: \(T_0\) between 500–1400 K (step of 100 K), \(N_0\) between \(10^{16} - 10^{20}\) cm\(^{-2}\), \(p, q\) between 0.5–1.4 (step of 0.1). The parameter uncertainties correspond to the 1σ confidence level\(^7\)

\(^7\) The 1σ confidence level is given by the \(\Delta \chi^2 = 1\) region, which corresponds to the confidence interval of each of the four parameters taken separately from the others (e.g., Bevington & Robinson 2003).

| Transition | \(\nu\) (GHz) | \(E_u\) (K) | HPBW (\(\circ\)) | \(\Delta v_{\text{peak}}\) (km s\(^{-1}\)) | FWHM (km s\(^{-1}\)) | Int. Intensity (K km s\(^{-1}\)) | Integrated Flux \((10^{-17} \text{ W m}^{-2})\) | \(R_{25}\%\) (AU) | \(R_{75}\%\) (AU) |
|------------|----------------|--------------|-----------------|-----------------|-----------------|-----------------|-----------------|----------------|----------------|
| CO J = 16–15 | 1841.345 | 751 | 11.1 | 5.3 | 8.2 | 2.8 ± 0.08 | 5.9 ± 0.2 | 7.68 | 8.72 |
| CO J = 10–9 | 1151.985 | 304 | 18.9 | 3.4 | 5.7 | 3.0 ± 0.09 | 4.5 ± 0.2 | 5.11 | 5.68 |
| CO J = 6–5 | 691.427 | 114 | 9.1 | 2.4 | 4.2 | 17.7 ± 0.9 | 1.32 ± 0.07 | 1.35 | 1.76 |
| CO J = 3–2 | 345.796 | 33 | 18.2 | 2.4 | 4.0 | 4.0 ± 0.6 | 0.15 ± 0.02 | 0.14 | 0.26 |
| [C II] | 1900.537 | 91 | 11.1 | 3.7 | 8.5 | 15.6 ± 0.4 | | | |

Notes: \(R_{25}\%\) and \(R_{75}\%\) indicate the radii encircling 25% and 75% of the emission as measured from the cumulative distribution (Figure 3).

\(^a\) Peak-to-peak velocity separation.

\(^b\) Panić et al. (2010).

\(^c\) Line flux predicted by the best-fit power-law model (Section 4).

\(^d\) Line flux predicted by the thermochemical model by Bruderer et al. (2012, Section 5).
The temperature radial gradient is well constrained thanks to the resolved velocity profiles (values of \( q < 0.6 \) are excluded at 3\( \sigma \) level). The column density is poorly constrained because the low-\( J \) lines (up to \( J = 16-15 \)) are optically thick (Bruderer et al. 2012).

The best-fit model is plotted in Figures 1 and 2 (blue solid line); the same power-law model reproduces the line velocity profiles and the overall shape of the rotational ladder. This simple model, however, produces too strong central absorption at low velocities (see discussion in Section 5).

Figure 3 (left) shows the cumulative distribution of the different CO transitions. The dot-dashed lines show the 25\% and 75\% limits and the corresponding radii are given in Table 1. The values of \( R_{25\%} \) and \( R_{75\%} \) indicate the radial distances in the disk where most of the line emission comes from: the \( J = 3-2 \) line emerges mainly from the outer disk (150–320 AU) while the highest-\( J \) line presented here emerges at intermediate radii (30–90 AU).

5. COMPARISON TO THERMOCHEMICAL MODELS

The knowledge of the temperature and column density radial distribution of warm gas is important for our understanding of the disk internal structure. How do these observational results compare with gas temperatures of thermochemical models? The (red) dashed lines in Figures 1 and 2 show the prediction of the standard thermochemical model of Bruderer et al. (2012) for the HD 100546 disk (corresponding to the representative model, discussed in Section 3 of that paper). The model results agree well with the observed line profiles. Specifically, it reproduces quantitatively the increasing width of the lines with increasing \( J \). It also provides a better fit to the profiles than the power-law model at low velocities because it accounts for the vertical structure of the disk. A related result of the full disk model is the decreasing emitting area of the lines with increasing \( J \) as a consequence of the thermal gradient in the radial direction: Bruderer et al. (2012) estimated that the 75\% of the \( J = 16-15 \) line emerges from a ring between 35–80 AU while the \( J = 3-2 \) line emerges from a ring between 70–220 AU, close to the inferred values.

The thermochemical model reproduces the overall shape of rotational ladder up to the mid-\( J \) lines (\( J = 24-23 \)), but it underestimates the flux of higher-\( J \) lines. As discussed in Bruderer et al. (2012, Sections 4 and 5) the flux of higher-\( J \) lines depends on the adopted \( \text{H}_2 \) formation rate. In Figure 2 we also show the fluxes of a model with a parameterized \( \text{H}_2 \) formation prescribed following Jonkheid et al. (2004) with \( T_{\text{term}} = 1600 \text{ K} \) (orange dot-dashed line). This model reproduces also the higher-\( J \) lines and it agrees well with the observed velocity profiles.

The value of \( q \) derived here indicates a steeper radial gradient of the gas temperature compared to the dust power-law index derived by interferometric observations at millimeter wavelengths (mean \( q_{\text{dust}} \sim 0.5 \), e.g., Andrews & Williams 2007; Hughes et al. 2008; Iella et al. 2009). The different radial gradient is likely due to the fact that the observed CO lines emerge from higher up in the disk compared to the millimeter dust emission which traces the disk mid-plane (where \( T_{\text{gas}} = T_{\text{dust}} \)). In these layers, the thermochemical models suggest high inner temperature (\( T_0 \), because of, e.g., photoelectric heating) and steep radial gradient (\( q \)) because of the thermal decoupling of gas and dust. This is shown in Figure 4 where the gas and dust temperature radial gradients are plotted for three different heights (\( z/r \)) in the disk relevant to the CO line formation. The power-law model overlaps with the thermochemical model at \( z/r = 0.2 \) in the inner region (\( r < 50 \text{ AU} \)) and at \( z/r < 0.25 \) in the outer disk (\( r > 100 \text{ AU} \)). Overall, our empirical gas temperature distribution provides a benchmark for future thermochemical models.

Another important test for the thermochemical models is the nature of the \([\text{C}\text{II}]\) emission on HD 100546. Based on the nondetection of \([\text{C}\text{I}]\), Bruderer et al. (2012) speculated that the disk lacks volatile carbon (i.e., carbon not locked up in refractory carbonaceous grains) compared to the ISM. One option is that CO ice has been transformed to \( \text{CH}_3\text{OH} \) and more complex ice species during the cold collapse phase of the cloud. Their model predicts the \([\text{C}\text{II}]\) emission associated with the disk to be almost an order on magnitude fainter than observed with PACS (after subtraction of the spatially extended emission). Our finding that most of the \([\text{C}\text{II}]\) flux measured with PACS and HIFI has a
non-disk origin (Figure 1 and Section 3.2) is consistent with this hypothesis.

6. CONCLUSIONS

In this Letter, we have used spectrally resolved observations of different CO lines to constrain the radial temperature gradient of the warm gas in the disk around HD 100546. The spectrally resolved CO lines show a velocity broadening consistent with the predictions of full thermochemical disk models (Bruderer et al. 2012). These observations therefore provide a new probe of the thermal decoupling of gas and dust as revealed by the high inner CO temperature ($T_0$) and steep temperature gradient ($q$). The HIFI [C II] spectrum confirms that the line flux measured with PACS is significantly contaminated by compact diffuse material.

Facility: Herschel

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