Warm CO in evolved stars from the THROES catalogue

I. *Herschel*-PACS spectroscopy of O-rich envelopes[★]

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ABSTRACT

In this work (Paper I), we analyse *Herschel*-PACS spectroscopy for a subsample of 23 O-rich and 3 S-type evolved stars, in different evolutionary stages from the asymptotic giant branch (AGB) to the planetary nebula (PN) phase, from the THROES catalogue. (C-rich targets are separately studied in Paper II). The broad spectral range covered by PACS ($\sim 55\text{--}210\ \mu\text{m}$) includes a large number of high- J CO lines, from $J = 14\text{--}13$ to $J = 45\text{--}44$ ($v = 0$), that allow us to study the warm inner layers of the circumstellar envelopes (CSEs) of these objects, at typical distances from the star of $\approx 10^{14}\text{--}10^{15}$ cm and $\approx 10^{16}$ cm for AGBs and post-AGB-PNe, respectively. We have generated CO rotational diagrams for each object to derive the rotational temperature, total mass within the CO-emitting region and average mass-loss rate during the ejection of these layers. We present first order estimations of these basic physical parameters using a large number of high- J CO rotational lines, with upper-level energies from $E_{\text{up}} \sim 580$ to 5000 K, for a relatively big set of evolved low-to-intermediate mass stars in different AGB-to-PN evolutionary stages. We derive rotational temperatures ranging from $T_{\text{rot}} \sim 200$ to 700 K, with typical values around 500 K for AGBs and systematically lower, ~ 200 K, for objects in more advanced evolutionary stages (post-AGBs and PNe). Our values of T_{rot} are one order or magnitude higher than the temperatures of the outer CSE layers derived from low- J CO line studies. The total mass of the inner CSE regions where the PACS CO lines arise is found to range from $M_{\text{H}_2} \sim 10^{-6}$ to $\approx 10^{-2} M_{\odot}$, which is expected to represent a small fraction of the total CSE mass. The mass-loss rates estimated are in the range $\dot{M} \sim 10^{-7}\text{--}10^{-4} M_{\odot} \text{ yr}^{-1}$, in agreement (within uncertainties) with values found in the literature. We find a clear anticorrelation between M_{H_2} and $\dot{M}$ vs. T_{rot} that probably results from a combination of most efficient line cooling and higher line opacities in high mass-loss rate objects. For some strong CO emitters in our sample, a double temperature (hot and warm) component is inferred. The temperatures of the warm and hot components are $\sim 400\text{--}500$ K and $\sim 600\text{--}900$ K, respectively. The mass of the warm component ($\sim 10^{-5}\text{--}8 \times 10^{-2} M_{\odot}$) is always larger than that of the hot component, by a factor of between two and ten. The warm-to-hot M_{H_2} and T_{rot} ratios are correlated and are consistent with an average temperature radial profile of $\propto r^{-0.5 \pm 0.1}$, that is, slightly shallower than in the outer envelope layers, in agreement with recent studies.

Key words. stars: AGB and post-AGB – circumstellar matter – stars: mass-loss – planetary nebulae: general – infrared: stars – stars: evolution

1. Introduction

The asymptotic giant branch (AGB) is one of the late stages in the evolution of low and intermediate mass stars ($1 M_{\odot} \lesssim M \lesssim 8 M_{\odot}$). At this phase, stars are very luminous ($\sim 10^4 L_{\odot}$) and cool, with effective temperatures ranging from $T_{\text{eff}} \sim 2000$ to 4000 K. The stellar radius of a typical AGB star is of about 1 AU, i.e. $R_{\star} \approx 10^{13}$ cm. AGB stars are dominated by an intense mass loss process with rates that range, typically, between 10^{-7} and $10^{-4} M_{\odot} \text{ yr}^{-1}$. For complete reviews see, for example, [Habing \(1996\)](#), [Herwig \(2005\)](#), [Höfner & Olofsson \(2018\)](#).

The vigorous mass loss generates a circumstellar envelope (CSE) of gas and dust around these evolved objects. The mass loss is thought to be produced by the combination of two mechanisms: pulsations and radiation pressure on dust ([Bowen 1988](#); [Simis et al. 2001](#)). Both mechanisms work together driving a

slow, dense stellar wind. The wind is strongly accelerated from the dust condensation region (at a few stellar radii, $\approx 10^{14}$ cm), reaching terminal velocities of about 5 to 25 km s⁻¹ at distances from the star of $\gtrsim 10\text{--}20 R_{\star}$. The temperature of the gas decreases along the CSE from 2000–2500 K, close to the stellar atmosphere, to ~ 1000 K in the dust condensation region, and progressively falling down to just a few tens of K in the most external envelope layers, at $\approx 10^{16}\text{--}10^{17}$ cm (e.g. [Decin 2012](#)).

The material ejected due to the mass loss process, is expected to enrich the interstellar medium (ISM) with stellar nucleosynthesis products. It is believed that about half of the elements heavier than Fe are formed in the AGB phase ([Herwig 2005](#)). The analysis of the molecular products found in the AGB CSEs is very useful to derive information on the nucleosynthesis history of the central star and to improve our current understanding of the complex circumstellar chemistry (e.g. [Millar 2016](#)).

The relative abundance of carbon and oxygen in the CSE completely determines the dominant chemistry of these envelopes. According to the ratio of carbon over oxygen atoms,

[★] *Herschel* is an ESA space observatory with science instruments provided by European-led Principal Investigator consortia and with important participation from NASA.

we identify envelopes with a carbon-rich ($C/O > 1$) or oxygen-rich ($C/O < 1$) chemistry, with a few objects (known as S-stars) showing C/O ratios very close to unity. This chemical branching is very important and depends on the nucleosynthesis processes that have taken place in the interior of these stars during their AGB evolution, which are basically determined by the mass of the progenitor star and its initial metallicity. All stars are born with a $C/O \sim 0.5$ and therefore O-rich. However, this chemical composition may change during their AGB evolution. According to theoretical models (Marigo et al. 2003; Karakas et al. 2009), low-mass progenitors ($M < 2 M_{\odot}$) remain as O-rich objects throughout the whole AGB evolution, while those stars with higher initial masses, between 2 and $4 M_{\odot}$, may become C-rich objects during the AGB phase due to the thermal pulses and convective processes (dredge-ups) that enrich the surface of the AGB star with carbon, produced as a result of nuclear reactions. Finally, the most massive objects (AGB stars with initial masses in the range $4 M_{\odot} < M < 8 M_{\odot}$) remain also O-rich throughout their evolution in the AGB as they do not produce so much carbon, instead they convert carbon into nitrogen via the CN cycle (in a process known as hot bottom burning).

After the AGB phase the convective envelope is expelled and the hot core starts to ionize the surrounding material. When the bulk of the gas in the CSE is ionized the object is recognized as a planetary nebula (PN), see Kwok (2005).

The transition phase between AGBs and PNe is called the post-AGB phase. It is a very fast ($\approx 10^3$ – 10^4 yr) phase when the shell, formed in the AGB phase, detaches from the central star and the spherical symmetry is usually broken due to the effect of the onset of fast bipolar or multi-polar winds (Balick & Frank 2002).

The CO molecule is one of the most abundant species found in these objects as it is quickly and easily formed from the O and C atoms present in the envelope and it is also the most stable at the typical conditions found in these envelopes, CO molecules develop strong rotational emission lines which are very useful to trace the physical properties of the molecular envelopes around evolved stars in different evolutionary stages, from the AGB to the PN phase.

The molecular emission of CO has been studied over the last decades mainly at mm and sub-mm wavelength ranges using the low- J transitions that trace outer ($>10^{16}$ cm) relatively cold (10–50 K) regions of the CSE (Bujarrabal 1999; Schöier & Olofsson 2001; Teyssier et al. 2006; Ramstedt et al. 2009). Studying the hotter layers of the envelope, presumably closer to the central star, traced by high- J CO transitions has only been possible with space telescopes like the Infrared Space Observatory (ISO; see, for example Justtanont et al. 2000) and in more recent times with *Herschel*, particularly, making use of PACS spectroscopy data (see, Groenewegen et al. 2011; Ueta et al. 2014).

Here, we analyse, in a uniform and systematic way, PACS spectroscopy data of a sample of O-rich (and a few S-type) evolved stars from the THROES catalogue (Ramos-Medina et al. 2018). We focus our study on the high-excitation rotational transitions of the CO molecule detected in these stars. In Sect. 2, a general description of our sample is provided. After that, in Sect. 3, we present the main characteristics of the PACS instrument and provide a brief description of the major data reduction steps. In Sect. 4 we show the principal observational results, including our measurements of the CO line fluxes. The rotational diagram (RD) analysis method used in this work and the results derived can be found in Sects. 5 and 6, respectively. The analysis of our results is presented in Sect. 7. Finally, in Sect. 8 we summarize our main conclusions.

2. Sample information

In this work we have studied 26 evolved stars at different evolutionary stages, from the AGB to PN phase, taken from the THROES catalogue (Ramos-Medina et al. 2018). In its current version, the THROES catalogue contains PACS spectroscopic cubes for a total of 114 low-to-intermediate mass evolved stars. In this study, we focus on non C-rich targets, with most of our sources being O-rich objects but also including a few S-type AGB stars (Table D.1). Sources with a dominant C-rich chemistry are studied separately by da Silva Santos et al. (in prep., Paper II). Our sources are grouped in five main categories as originally defined in the THROES catalogue: classical O-rich and S-type AGB stars, OH/IR stars (strong far-IR emitters with intense OH maser lines, typically late-AGB or early post-AGB stars heavily obscured by dust at optical wavelengths), post-AGB objects, and PNe. For this study, we have selected objects with a minimum of three CO transitions detected with a ratio of $S/N > 3$, a total of 26 out of 66 non C-rich targets in the THROES catalogue.

In Fig. 1 we present IRAS fluxes and colours of the sources of our sample in comparison with the rest of objects (C-rich or CO non-detections of any chemical type) contained in the THROES catalogue. IRAS colours in this diagram are defined as: $[12] - [25] = 2.5 \log_{10} \frac{IRAS_{25}}{IRAS_{12}}$ and $[25] - [60] = 2.5 \log_{10} \frac{IRAS_{60}}{IRAS_{25}}$. In the colour-colour diagram, the sources included in the THROES catalogue follow a well-known evolutionary sequence, with the AGBs located at the bottom left region (boxes: I, II, IIIa and VII) and the post-AGBs and PNe occupying the upper right area (boxes: V and VIII); more details can be found in van der Veen & Habing (1988). We note that the only OH/IR star located close to other PNe in region V is OH 231.8+4.2, which is a peculiar AGB star with a massive outflow with physical and chemical particularities uncommon for the AGB stage but approaching those of post-AGB objects (e.g. Alcolea et al. 2001; Sánchez Contreras et al. 2015).

All the objects of our sample except two, IRAS 17347-3139 and NGC 6537, have previous estimations of the mass loss rate but using low- J CO lines detected in the sub-millimetre and millimetre ranges (see Table D.2). Only for six objects namely, NML Tau, TX Cam, R Dor, R Cas, W Hya and W Aql, the mass loss rates provided come from recent works (Danilovich et al. 2014; Khouri et al. 2014; Maercker et al. 2016; Van de Sande et al. 2018) which are based on detailed non-local thermal equilibrium (non-LTE) radiative transfer models which make use of a combination of different sets of CO lines taken from several telescopes and including HIFI and PACS observations that, eventually, cover CO rotational lines up to $J = 24$ –23. We have paid particular attention to the mass loss rates estimations derived in these works in order to test the results obtained with the rotational diagram method, used in this paper.

3. Observations and data reduction

PACS (Poglitsch et al. 2010) is an instrument onboard *Herschel* (Pilbratt et al. 2010) with photometric and spectroscopic capabilities in the FIR wavelength region. The PACS spectrometer covers the wavelength range from 51 to $210 \mu\text{m}$ in two different channels that operate simultaneously in the blue (51– $105 \mu\text{m}$) and red (102– $220 \mu\text{m}$) bands. The Field of View (FoV) covers a $47'' \times 47''$ region in the sky, it is structured in an array of 5×5 spatial pixels (“spaxels”), each spaxel is a $9.4'' \times 9.4''$ square. PACS provides a resolving power between 5500 and 940 (i.e.

Fig. 1. IRAS colour-colour diagram (*left*) and 100 μ m flux vs. $[12] - [25]$ IRAS colour (*right*) of the THROES targets with good quality IRAS data (Quality Flag = 3) in the 12, 25, 60 and 100 μ m bands. The colour-colour diagram is divided in different boxes where sources with common characteristics and evolutionary stages are located (see [van der Veen & Habing 1988](#), for details). Objects with CO line detections, studied in this work, are highlighted using the symbol and colour code shown in the figure. In the rest of the plots presented throughout this paper, AGBs, OH/IRs, post-AGBs and PNe are coloured and symbol-coded as indicated in this figure.

a spectral resolution of 55–320 km s^{-1}) at short and long wavelengths, respectively, and the point spread function (PSF) of the PACS spectrometer ranges from $\sim 9''$ in the blue band to $\sim 13''$ in the red band. The PSF is described in [da Silva Santos \(2016\)](#) and [Bocchio et al. \(2016\)](#). Complete details about PACS instrument can be found in the PACS Observer’s Manual¹.

In this work we have used one-dimensional (1D) PACS spectra, integrated over the emitting source, taken from the THROES catalogue ([Ramos-Medina et al. 2018](#)). THROES is a web-based catalogue that contains fully reduced PACS spectra, in 3D cubes structure (FITS files) and 1D spectra format (FITS and CSV files), for 114 low-to-intermediate mass evolved stars, covering a range of evolutionary stages from the AGB to the PN phase. The THROES catalogue is public and can be accessed online².

The main goal of the THROES project was the production of enhanced PACS spectroscopic data through the systematic careful interactive reprocessing, for full science exploitation of the spectra. Apart from the standard data reduction steps (most of them) common to the pipeline, some extra corrections were added such as: flat-field, background correction and other post-processing corrections applied in particular cases to extract the science-ready 1D PACS spectra from the 3D data cubes. In this process, the extent of the sources and their precise position in the FoV of PACS were taken into account. Particular attention was given to the mispointed cases (those objects not perfectly centred on the central spaxel of the PACS field of view). Full details on the data reduction process of the THROES targets can be found in [Ramos-Medina et al. \(2018\)](#).

The complete 1D spectra reported here are formed by four individual sub-spectra that cover four different wavelength sub-ranges resulting in a final spectral coverage that ranges from 55 to 95 μ m (blue band) and from 105 to 190 μ m (red band). All the objects included in this work have a full spectral coverage except RR Aql and T Cep, whose 1D PACS spectra cover only two of the spectral subranges: from 55 to 73 μ m and from 105 to 147 μ m.

4. Observational results

In Figs. 2 and 3 we display the continuum subtracted PACS spectra of the sources studied in this paper from 55 to 95 μ m and from 110 to 190 μ m, respectively. The continuum was fitted using a non-parametric method after identifying the line-free regions of the spectrum for each target.

The sources are sorted in Figs. 2 and 3 attending to their classification with the O-rich AGBs at the top, followed by S-type stars, OH/IR stars, post-AGB stars and PNe. Inside each group, the objects are sorted attending to the effective temperature of the central star, with the coolest object at the top and the hottest one at the bottom. The way the objects have been sorted evidences how different the spectra are along the different evolutionary stages from AGB phase to the PN stage. While the spectra of the envelopes around AGB stars show hundreds of molecular emission lines the density of emission lines in post-AGB objects is clearly lower. Finally, the most evolved objects, with highest temperatures of central stars, the PNe, show intense atomic emission lines in their envelopes and a lack of molecular features compared to the AGBs.

Rotational CO transitions in the ground vibrational state ($v = 0$) are the most prominent molecular lines found in all the spectra. We have detected and measured the integrated flux of CO $v = 0$ rotational lines with high- J levels, up to $J = 42$ ($E_{\text{up}} \sim 4700$ K). We have checked that, as expected, the resolving power of PACS (of a few 100 km s^{-1}) does not allow us to spectrally resolve the line profiles, which are expected to have full widths at half intensity similar to the terminal expansion velocity of the envelopes, $FWHM \sim 20\text{--}40$ km s^{-1} in the majority of our sample. The PACS CO line profiles are also unresolved for a few post-AGB objects and PNe in our sample that are known to have fast outflows sampled by low- J transitions, that is OH 231.8+4.2 ([Alcolea et al. 2001](#)).

Apart from CO, we have also detected molecular emission lines from H₂O, including orto- and para- configurations, OH, HCN or SiO amongst others. Some of these lines have been reported for some objects of our subsample in (e.g. [Danilovich et al. 2014](#); [Maercker et al. 2016](#)). Atomic lines such

¹ herschel.esac.esa.int/Docs/PACS/pdf/pacs_om.pdf

² <https://throes.cab.inta-csic.es>

Fig. 2. PACS continuum subtracted spectra of our sample in the 55–75 μm range. The ^{12}CO rotational lines are indicated by vertical dotted lines (see Table D.4). The upper-level rotational quantum number J_{u} of a few selected CO transitions are shown as a reference. The sources are sorted from top to bottom in these five groups: AGBs, S-type stars, extreme OH/IR stars, post-AGBs, and PNe. Within each category, targets are ordered based on the stellar effective temperature from the coolest source to the hottest one.

Fig. 3. The same as in Fig. 2 but covering the spectral range from 110 to 190 μm .

Fig. 4. *Top:* integrated flux of the CO $J = 15-14$ transition at $173.6\mu\text{m}$ ($F_{\text{CO } 15-14}$) against the IRAS $100\mu\text{m}$ flux. Targets with no PACS data beyond $\sim 145\mu\text{m}$ (i.e. not covering this CO transition; RR Aql and T Cep – see Fig. 3) or with bad quality (Quality Flag $\neq$ 3) IRAS₁₀₀ data (OH 26.5+0.6) are excluded. *Middle:* fluxes of the CO $J = 15-14$ transition and the adjacent continuum (PACS₁₇₀). In this diagram, OH 26.5+0.6 is included. *Bottom:* line-to-continuum ($F_{\text{CO } 15-14}/\text{PACS}_{170}$) flux ratio against the IRAS colour $[12]-[25]$.

as OI ($63\mu\text{m}$), OIII ($88\mu\text{m}$), NII ($122\mu\text{m}$) and CII ($158\mu\text{m}$) are also identified in post-AGBs and PNe, but not in AGBs. Finally,

broad dust emission features associated to forsterite at $69\mu\text{m}$ are also found in 4 objects: NGC 6537, NGC 6302, OH 231.8+4.2 and OH 26.5+0.6. Previous detections of forsterite in evolved stars with *Herschel* are shown, for example, in de Vries et al. (2015) and Blommaert et al. (2014). The integrated fluxes of the CO rotational emission lines detected in our sample are shown in Table D.4.

Certain CO rotational lines are known to be blended with transitions by other abundant species that lie within the same PACS spectral resolution element. We have identified, for example, the blend of CO ($J = 23-22$) with o-H₂O (414–303), and that of CO ($J = 22-21$) with the ¹³CO ($J = 23-22$) and HNC ($J = 28-27$) transitions. Line blends were excluded in our RD analysis, but these lines are listed and integrated fluxes are reported in Table D.4 for completeness. In this table, we also list the lines that present a poor estimation of the underlying continuum level, although they have not been used for the rotational diagram analysis given their very large flux error bars. Finally, we note that the CO ($J = 27-26$) and ($J = 26-25$) transitions are missing for all targets since there is a gap in the $95-102\mu\text{m}$ region of the PACS detector where these lines lie. The errors in the CO line fluxes are derived using the error associated to the fitting, estimated using the rms value of the continuum adjacent to the line, and assuming a flux calibration error of 15%.

In Fig. 4 we compare the integrated flux of the CO ($J = 15-14$) transition at $173.6\mu\text{m}$ ($F_{\text{CO } 15-14}$) with other observational parameters, in particular, with the IRAS $100\mu\text{m}$ flux (IRAS₁₀₀), the PACS continuum at $170\mu\text{m}$ (PACS₁₇₀), i.e. near the CO ($J = 15-14$) line, and the $[12]-[25]$ IRAS colour. As expected, there is a correlation between the CO line strength and the IRAS₁₀₀ and PACS₁₇₀ continuum fluxes, which confirms that objects with stronger molecular emission show, typically, stronger continuum emission from dust as well. Of course, in addition to an intrinsic relation between these two observational parameters, there is also a dependence with the distance to the sources, which is partially responsible of the observed relation. The scatter of the points is significantly larger in the $F_{\text{CO } 15-14}$ vs. IRAS₁₀₀ distribution, which partially reflects the variability of the majority of the targets (pulsating AGB stars) given that PACS and IRAS observations were obtained at different epochs, as well as different instrument calibration uncertainties, background contamination sources, beam size and pointing, etc. These effects are discussed for the whole sample of the THROES catalogue in Ramos-Medina et al. (2018). We find an anticorrelation between the line-to-continuum ($F_{\text{CO } 15-14}/\text{PACS}_{170}$) ratio and the IRAS $[12]-[25]$ colour, which are both distant-independent parameters. In general, we find that the ratio between the molecular emission and the dust emission is higher in less evolved objects than in the most evolved ones.

5. CO emission analysis: rotational diagrams (RD)

The CO rotational lines provide a fundamental diagnostic of the physical conditions of the molecular gas. As a first approximation, we calculated the rotational population diagrams of the CO (J_u-J_l) $v = 0$ transitions observed with PACS assuming optically thin emission under LTE conditions. We have used the approach presented by Justanont et al. (2000), where the total flux observed is used to derive the total mass of the CO-emitting volume adopting the distance to the source indicated in Table D.2.

The concept of the RD analysis is very simple, see Goldsmith & Langer (1999). Assuming LTE, the population of each level N_u can be described by a single rotation temperature

T_{rot} , which is expected to be the same as the kinetic temperature, and given by the Boltzmann distribution:

$$N_u = \frac{N_{\text{CO}}}{Q(T_{\text{rot}})} g_u e^{-E_u/(\kappa T_{\text{rot}})}, \quad (1)$$

where N_{CO} is the total number of CO molecules in the emitting volume, $Q(T_{\text{rot}})$ is the rotational partition function and g_u are the statistical weights for each upper level. Equation (1) can be rewritten in the following form:

$$\ln\left(\frac{N_u}{g_u}\right) = \ln\left(\frac{N_{\text{CO}}}{Q(T_{\text{rot}})}\right) - \frac{E_u}{\kappa T_{\text{rot}}} - \ln C_\tau, \quad (2)$$

where C_τ is the opacity correction term defined as $C_\tau = \frac{\tau_\lambda}{1-e^{-\tau_\lambda}}$ by, e.g., Goldsmith & Langer (1999). The left hand side of Eq. (2) can be estimated using the relation between the observed flux of a single line and the number of molecules at the upper level (N_u):

$$N_u = \frac{4\pi F \lambda_{\text{ul}} d^2}{A_{\text{ul}} h c}, \quad (3)$$

where F is the integrated line flux, λ is the rest wavelength of the transition, d is the distance to the source, A_{ul} is the Einstein's spontaneous emission coefficient associated to the transition, h is the Planck's constant and c represents the speed of light.

In our RDs we represent $\ln\left(\frac{N_u}{g_u}\right)$ against $\frac{E_u}{\kappa}$ and we apply a linear regression that allow us to obtain T_{rot} (derived from the slope) and N_{CO} (estimated from the intercept in the y-axis) following Eq. (2).

With the values of N_{CO} and T_{rot} derived from this first fitting we estimate those of τ and C_τ from Eq. (4) in Sect. 5.1. This initial estimation is used to obtain new values of $\ln\left(\frac{N_u}{g_u}\right)$ applying the correction shown in Eq. (2). Then we can apply a new linear fit to this new set of values to derive the so-called opacity corrected values for T_{rot} and N_{CO} that are the ones adopted for the rest of the analysis. We want to highlight that the opacity correction derived is moderate being the τ values estimated for each object close to 1 (see Sect. 5.1). Very high values of τ would lead to unreliable results from the RD analysis, see Goldsmith & Langer (1999) for details.

5.1. Opacity correction

The optical depth (τ_λ) of a CO line is given by:

$$\tau_\lambda = \frac{A_{\text{ul}} \lambda_{\text{ul}}^3 N_u^{\text{col}}}{8\pi \nu_{\text{exp}} \sqrt{\pi} (2 \sqrt{\log 2})} \times (e^{(hc/(\lambda_{\text{ul}} \kappa T_{\text{rot}}))} - 1), \quad (4)$$

where N_u^{col} is the column density of CO in the upper level of the transition.

We need an estimation of T_{rot} and $N_{\text{CO}}^{\text{col}}$ to calculate τ . T_{rot} is directly extracted from the RDs and $N_{\text{CO}}^{\text{col}}$ is derived from the total number of CO molecules, N_{CO} , through the following, simplified, equation: $N_{\text{CO}}^{\text{col}} = \frac{N_{\text{CO}}}{\pi r_{\text{CO}}^2}$. Where r_{CO} represents the characteristic radius of the region where the bulk of the CO emission is produced.

The value of r_{CO} is one of the main sources of uncertainty to compute the optical depth and the subsequent opacity correction term. Unfortunately, as mentioned in Sect. 3, the inner envelope layers where the CO PACS lines are produced are unresolved or barely resolved in the PACS spectroscopy cubes for most of the sources given the large PSF ($\sim 9''$ – $13''$) and pixel size ($9''.4$) of

the instrument (see Sect. 3). Therefore, the value of r_{CO} needs to be adopted based on several criteria. These criteria are described in detail in Appendix B, and a summary is offered in the following paragraphs.

For AGB stars, an estimate of r_{CO} is obtained by comparing the values of T_{rot} deduced from our analysis, ~ 200 – 700 K, with the radial temperature distribution $T(r)$ in the envelopes of a number of AGB stars with detailed non-LTE excitation and radiative transfer studies of their CO emission. The gas temperature can be up to 2000 K near the dust condensation radius ($\sim 10^{14}$ cm), and decreases gradually towards the outermost layers following, approximately, a power-law of the type $\sim 1/r^\alpha$, with $\alpha \sim 0.5$ – 1.0 , see Van de Sande et al. (2018), Maercker et al. (2016), Danilovich et al. (2014), Khouri et al. (2014). For our sample, we deduce a range of values of r_{CO} from about 2×10^{14} cm to $[2\text{--}4] \times 10^{15}$ cm, with the highest mass-loss rate objects requiring the largest values of r_{CO} . The values of r_{CO} adopted for our targets are given in Table D.3.

The CO column densities derived from our RD analysis adopting a range of r_{CO} from $\sim 10^{14}$ to $\sim 10^{15}$ cm are moderate, $N_{\text{CO}}^{\text{col}} < \sim 10^{19}$ cm $^{-2}$, resulting in line optical depths of the order of ~ 0.9 , and even lower in some cases, for the CO $J = 14 \rightarrow 13$ transition, which is the line with the largest opacity in our study. For AGBs, we have tuned r_{CO} to a value slightly larger than the radius of the wind layer where $\tau_{J=14 \rightarrow 13} \sim 1$; the latter is indeed the deepest region of the envelope observationally accessible, because of the almost null escape probability ($1/C_\tau = \frac{(1-e^{-\tau})}{\tau} \rightarrow 0$) from much deeper, optically thicker ($\tau \gg 1$) layers of the wind.

Not only for the AGB stars but also for the OH/IR stars, we find that values of the radius around $r_{\text{CO}} \sim [2\text{--}4] \times 10^{15}$ cm result in line optical depths close to, but smaller than, unity (typically $\tau_{J=14 \rightarrow 13} \sim 0.5$ – 0.7) that result in moderate C_τ opacity correction factors. For all the objects studied in this work, the opacity correction is typically negligible for lines higher than $J = 19$ – 18 .

Unlike for AGBs and OH/IR stars, for post-AGBs/PNe there are no theoretical or observationally constrained temperature profiles of the molecular gas component available in the literature. For these targets, we find that $\tau_{J=14 \rightarrow 13}$ approaches a value of ~ 1 at distances of $r_{\text{CO}} \sim 1 \times 10^{16}$ cm, which therefore have been taken as a lower limit to the radius of the CO emitting volume detected with PACS. The PACS spectroscopy cubes indeed show extended, partially resolved nebulosities consistent with a linear diameter of $\lesssim [1\text{--}2] \times 10^{17}$ cm (da Silva Santos 2016), in some of these cases. Using additional information on the molecular envelope extent from the literature and aiming to treat the sources as homogeneously as possible, we have adopted a common value of $r_{\text{CO}} = 6 \times 10^{16}$ cm for the 5 post-AGBs/PNe in our sample, resulting in column densities of $N_{\text{CO}} \lesssim 1\text{--}5 \times 10^{17}$ cm $^{-2}$ and small line optical depths of $\tau_{J=14 \rightarrow 13} \sim 0.02$ – 0.07 .

It must be noted that, in addition, we have completed our analysis by systematically exploring a range of radii around the value of r_{CO} adopted in each case to investigate the impact of this uncertain parameter in our results (see Fig. C.1). As expected, the smaller the r_{CO} , the larger the opacity correction, which results in lower values of T_{rot} and larger values of N_{CO} . We note that after applying the C_τ correction, the slope of the RD increases, as a direct result of the frequency-dependence of C_τ and the typical values of T_{rot} in our sample, see Appendix B. For example, in AGBs and OH/IR stars, values of $r_{\text{CO}} \gtrsim 5 \times 10^{15}$ cm always result in negligible opacity corrections, whereas for values of $r_{\text{CO}} \lesssim 8 \times 10^{14}$ cm the opacity becomes larger than one for most targets, except for the sources with the lowest mass-loss rates ($\dot{M} \sim 10^{-8} M_\odot \text{ yr}^{-1}$, see

Table D.2) where the CO lines remain optically thin at these radii.

6. Results

6.1. Rotational temperatures and total emitting mass of H_2

The CO RDs of our targets, from which we derive the rotational temperature (T_{rot}) and the total number of CO molecules (N_{CO}) in the emitting volume, are shown in Figs. 5a–c. For most objects, the RDs include CO transitions with upper-level energies that range from $E_{\text{up}} \sim 580$ K to $E_{\text{up}} \lesssim 2500$ K and are well fitted using a single temperature component. The single-fit rotational temperatures obtained range from ~ 200 K (NGC 6537) to ~ 700 K (π Gru), with an average value of $T_{\text{rot}} \sim 450$ K.

For a number of strong CO emitters (NML Tau, χ Cyg, W Aql, NML Cyg and IRAS 17347-3139) transitions with upper-level energies of up to $E_{\text{up}} \sim 5000$ K are also detected. In these cases, the data points in the RD over the full E_{up} covered are not well reproduced by a single straight-line fit. A double-slope in the RD is expected if a range of temperatures occur along the line of sight.

We have formally tested that a double-slope fit is indeed most appropriate in these cases using statistical tools for model selection: F statistics and Bayesian Information Criterion (BIC), implemented in R programming language in the *strucchange*³ package (see Paper II for more details). We refer to the CO emitting regions with the lowest and highest T_{rot} values derived from the double-fit as the “warm” and “hot” CO components, respectively (Figs. 5a–c). The rotational temperatures of the warm and hot components are in the range ~ 370 – 480 K and ~ 570 – 900 K, respectively. As expected, the values of T_{rot} obtained from a single-fit to the RDs are intermediate to those of the warm and hot components.

The total number of CO molecules in the emitting volume, N_{CO} , derived from the RDs has been converted to total mass of molecular hydrogen using:

$$M_{H_2} = \frac{N_{\text{CO}}}{\chi_{\text{CO}}} m_{H_2}, \quad (5)$$

where m_{H_2} is the mass of a molecule of hydrogen ($m_{H_2} = 2.0159$ a.u. $= 3.3475 \times 10^{-24}$ g) and χ_{CO} is the CO-to- H_2 fractional abundance, assumed to be 2×10^{-4} for O-rich objects (Ramstedt & Olofsson 2014) and 6×10^{-4} for S-type stars (Ramstedt & Olofsson 2014; Danilovich et al. 2014).

The resulting values of M_{H_2} and T_{rot} are listed for each target in Table D.3, together with a few other relevant parameters (such as the adopted r_{CO} for the moderate opacity correction applied, Sect. 5.1). In Fig. 6 we show the M_{H_2} and T_{rot} values for each target, with and without the opacity correction, and the final histogram distributions.

The single-fit values of the total mass of the CO-emitting volume range between $M_{H_2} \sim 3 \times 10^{-6} M_{\odot}$ (X Her) and $\sim 5 \times 10^{-2} M_{\odot}$ (IRAS 17347-3139), with an average value of $M_{H_2} \sim 4 \times 10^{-3} M_{\odot}$. The opacity correction applied in all cases is small-to-moderate, which results in a mass-correction factor less than 20% in most sources. The source with the largest opacity correction (of a factor ~ 1.5) is NML Cyg, the AGB star with the largest M_{H_2} , and highest mass-loss rate, in our sample (Table D.2).

The mass of the warm CO component is always larger than the mass of the hot component. For the warm component, these

values vary from $M_{H_2} \sim 1.3 \times 10^{-5}$ to $7.8 \times 10^{-2} M_{\odot}$, and for the hot between 3.7×10^{-6} and $1.6 \times 10^{-2} M_{\odot}$. The warm-to-hot M_{H_2} and T_{rot} ratio, and their relation, is further examined in Sect. 7.

We have investigated if there are any trends between T_{rot} and M_{H_2} , derived for our RD analysis, and other observational parameters, such as the terminal expansion velocity of the envelope (v_{exp}) and the strength of the CO ($J = 15$ – 14) transition (Fig. 7). First, we notice that objects in the most advanced stages of the evolution, namely, post-AGBs and PNe, systematically have the lowest temperatures, $T_{\text{rot}} \sim 200$ – 300 K, and the highest masses, $M_{H_2} > 0.01 M_{\odot}$ (see also Fig. 6). IRAS 17347-3139 is the only object with an exceptionally large T_{rot} for its class. The distribution of T_{rot} and M_{H_2} for post-AGB and PNe is also much narrower than for AGBs and OH/IR. The latter show a broad range of $T_{\text{rot}} \sim 200$ – 700 K and $M_{H_2} \sim 10^{-6}$ – $10^{-3} M_{\odot}$. This segregation of the sources exists before and after the opacity correction has been applied; the opacity correction is indeed marginal for post-AGBs and PNe (grey symbols in Fig. 6). The observed bias in favour of massive post-AGB/PNe could reflect that, in our sample, post-AGB/PNe are on average more distant ($d > 1$ kpc) than AGBs and OH/IRs stars, which hampers CO line detections in the less massive post-AGB/PNe.

We observe an anticorrelation between M_{H_2} and T_{rot} (Fig. 7, top-left panel). This is most clearly noticed amongst AGB and OH/IRs, which are more numerous and cover a broader range of T_{rot} and M_{H_2} values, but it is also followed by post-AGB/PNe. We note that for objects for which a double- T_{rot} component has been identified (NML Tau, χ Cyg, W Aql, NML Cyg and IRAS 17347-3139), both the double- and the single-fit values (connected with dashed lines in Fig. 7, top-left panel) follow the trend. The object IRAS 17347-3139 is an outlier, since it has a much larger T_{rot} than anticipated based on the overall properties of the rest of our sample. This object is known to be at the earliest stages of the post-AGB evolution and making a fast transition to the PN phase at present (Table D.2, see Gómez et al. 2005; Tafaya et al. 2009).

For AGBs and OH/IRs stars, there is also an evident linear correlation between M_{H_2} and the terminal expansion velocity of the envelope (from the literature – Table D.3). As we will see in Sect. 7.4, this is linked to an analogue $\dot{M}$ -to- v_{exp} relation, which is known to exist based on previous low- J CO studies of AGB CSEs (e.g. Danilovich et al. 2015) and that we corroborate in this work using higher- J CO lines. The post-AGB objects and PNe in our sample, however, show very similar values of the mass over a the full range of velocities.

As expected, the integrated flux of the CO lines correlate with the total mass of the CO-emitting volume and, as we will see later, with the average mass-loss rate of the envelopes. As an example we show this relation for the CO $J = 15$ – 14 transition ($E_{\text{up}} \sim 660$ K) in Fig. 7 (bottom-left). There is a significant scatter in the line flux vs. M_{H_2} relation since the latter also depends on the excitation temperature (T_{rot}), the velocity field in the envelope, the optical depth, etc. (Sect. 5).

Finally, we investigated if a correlation exist between the CO $J = 15$ – 14 line integrated flux normalized to the underlying $\sim 170 \mu\text{m}$ -continuum observed with PACS ($F_{\text{CO } 15-14}/\text{PACS}_{170}$) and the parameters derived from the RD analysis. The strongest correlation is found with T_{rot} (Fig. 7, bottom-right), which is somewhat expected since the mass and the distance dependence is removed in the line-to-continuum flux ratio. The relation between $F_{\text{CO } 15-14}/\text{PACS}_{170}$ with M_{H_2} (not shown) has a much larger scatter and suggests a certain anticorrelation (given that T_{rot} anticorrelates with M_{H_2} in our sample).

In Sect. 7 we further discuss the observed trends.

³ <https://cran.r-project.org/web/packages/strucchange/index.html>

Fig. 5. RDs of CO for our targets (continues in 5b and 5c). For each source, the values of T_{rot} and M_{H_2} derived from the fits (solid lines) as well as the characteristic radius of the emitting envelope layers adopted (r_{CO}) are shown (Sect. 5). The errors of T_{rot} and M_{H_2} represent the uncertainty of the fit considering the error bars of the individual points, which include formal errors due to the noise and absolute flux uncertainty of the PACS spectra. For a few sources, a double component fit was necessary. For these cases, the values of T_{rot} and M_{H_2} for the so-called warm (blue) and hot (red) components are also indicated.

6.2. Mass-loss rate

Using the values of the total emitting mass, we calculate the mass-loss rates ($\dot{M}$) for each source in a simplified manner dividing the total mass by the crossing time of the CO-emitting layers, that is:

$$\dot{M} = \frac{M_{H_2} v_{exp}}{r_{CO}}, \quad (6)$$

Apart from M_{H_2} , derived from the RDs, we need to adopt a value for the expansion velocity (v_{exp}), which has been taken from literature, as well as for the characteristic radius of the CO emitting region, for which we use the same value used for the estimation of the opacity correction, r_{CO} . The values of $\dot{M}$ are given in Table D.2.

In Sect. 5, we already mentioned the uncertainties associated to the adoption of a particular linear radius for the emitting region of each source and the importance of exploring a wide range of values to determine a reasonable estimation of the opacity correction and, thus, of M_{H_2} . The same kind of analysis is even more important now, as the impact of r_{CO} in the mass-loss

rate estimation is larger than in the calculation of the opacity correction (it affects M_{H_2} but also directly $\dot{M}$ as $\sim 1/r_{CO}$). Another uncertainty arises in v_{exp} , however, this parameter is rather well known (from previous works), to an accuracy of $\sim 10\text{--}20\%$ typically.

In Fig. C.2, we show, for every object, the different values of $\dot{M}$ and T_{rot} that correspond to three different values of the radius around the adopted value. For each source, we have also plotted a grey region that represents the broad interval of mass-loss rates found in the literature. The latter are usually derived from the analysis of low- J CO lines and, therefore, they represent the average mass-loss rate in the outer envelope layers. These values of $\dot{M}$ from the literature have been re-scaled after matching the expansion velocity (v_{exp}), the distance (d) and the relative abundance of CO (χ_{CO}) to the values adopted here, which is needed for a proper comparison with our estimates of $\dot{M}$. The values of the mass-loss rates reported in the bibliography for each object are displayed in Table D.2 together with the associated interval range of mass-loss rates after scaling and relevant references. To our knowledge, for IRAS 17347-3139 and NGC 6537 there are no previous estimates of the gas mass-loss rate in the literature.

Fig. 5. continued.

Our estimates of the mass-loss rates are shown in Fig. 8 plotted against the rotational temperature, the expansion velocity, and the CO($J = 15-14$) line strength to explore any trends that may be present. In the $\dot{M}$ vs. T_{rot} diagram we also include the mass-loss rates associated to the warm and hot component for objects with a double-slope in their RDs. There is an anti-correlation between $\dot{M}$ and T_{rot} , which was expected based on a similar trend observed directly between M_{H_2} and T_{rot} (Fig. 7). This trend together with the clear correlation between $\dot{M}$ and v_{exp} and, more scattered, trend with $F_{CO\,15-14}$ are briefly discussed in Sect. 7.

7. Analysis and interpretation of the results

In this section, we analyse and discuss the results obtained from the RDs as well as the correlations found between different magnitudes.

7.1. Rotational temperature and total mass

For most of our sources, a single- T_{rot} component was sufficient to obtain a good fit of the CO RD, leading to single-fit rotational temperatures and total (H_2) masses of the CO-emitting region of $T_{rot} \sim 200-700$ K and $M_{H_2} \sim 3 \times 10^{-6} - 5 \times 10^{-2} M_\odot$, respectively (Sect. 6).

The rotational temperatures of a few 100 K derived in this work using CO-PACS data ($J_u \sim 14-27$, and up to $J_u = 40$ lines in some cases) are clearly larger than the typical values of $T_{rot} \sim 10-100$ K found from CO low- J line studies (most commonly using $J_u < 4$ lines at mm and sub-mm wavelengths) in the external layers of the CSE around evolved stars, at $\sim 10^{16}-10^{17}$ cm from the center (e.g. Teyssier et al. 2006, and references therein). This corroborates that, as anticipated, the CO-PACS lines sample the warm, presumably inner, regions of the CSEs, probably at a typical/average distance from the central star of about $\sim 10^{15}$ cm for AGB stars (e.g. Danilovich et al. 2014).

We find that the total mass of the warm inner layers where the PACS CO ($J_u > 14$) lines mainly arise is typically a factor $\sim 100-1000$ lower than the masses deduced from low- J CO line studies in the literature, reinforcing the idea that CO PACS lines sample mainly the inner part of the envelopes, which contains a small fraction of the total envelope mass.

For a total of five targets in our sample (NML Tau, π Gru, W Aql, χ Cyg and IRAS 17347-3139), the RD diagram shows a double slope and, thus, a double- T_{rot} fit is most appropriate. Deviations from a single straight line fit of the RDs, most likely denoting a temperature stratification along the line of sight (see below), are not uncommon and have been previously found in a number of AGB and post-AGB CSEs using ISO and/or SPIRE

Fig. 5. continued.

 Fig. 6. Values of T_{rot} and M_{H_2} from our CO rotational diagram analysis (single fit; Sect. 6) before and after applying the opacity correction (grey and coloured symbols, respectively).

CO spectra (e.g. Justtanont et al. 2000; Wesson et al. 2010; Matsuura et al. 2014; Cernicharo et al. 2015; Cordiner et al. 2016).

The rotational temperatures and masses of the hot and warm components of these five objects are displayed in Fig. 7 (together with the single-fit T_{rot} and M_{H_2} values derived for the whole sam-

ple). The mass of the warm component is always larger (by a factor 2–10) than that of the hot component. Adopting a constant mass-loss rate and a gas temperature that decreases with the distance, the difference between the mass of the warm and hot component suggests a CO-emitting volume smaller for the hot component than for the warm one.

Fig. 7. Relation between M_{H_2} and T_{rot} derived from our CO RD analysis and other magnitudes. *Top-left:* M_{H_2} vs. T_{rot} . For objects (a total of five) with a double- T_{rot} component, both the single-fit and double-fit values are connected with dashed lines for an easier identification. *Top-right:* values of M_{H_2} (single-fit) vs. v_{exp} taken from the literature. *Bottom panels:* integrated fluxes of CO ($J = 15-14$) line vs. M_{H_2} (left) and the same line normalized to its adjacent continuum vs. T_{rot} (right).

We compare in detail the hot-to-warm M_{H_2} and T_{rot} ratios in Fig. 9. We find that the mass and temperature ratios are well correlated and follow approximately a power-law function. For AGB CSE with an inverse-square density profile, the latter is indeed expected if the temperature stratification within the emitting layers is described by a power-law function, $T(r) \sim 1/r^\alpha$. This is because, in this case, the total mass within a given CO-emitting volume is roughly proportional to its radius ($M_{\text{H}_2} \propto r$) and, therefore, it is easy to derive that:

$$\frac{T_{\text{rot}}^{\text{hot}}}{T_{\text{rot}}^{\text{warm}}} \sim \left(\frac{M_{\text{H}_2}^{\text{hot}}}{M_{\text{H}_2}^{\text{warm}}} \right)^{-\frac{1}{\alpha}}, \quad (7)$$

Fitting a power-law function to the set of points corresponding to our AGB stars⁴, we obtain $\alpha = 0.5 \pm 0.1$. This value is at the low end of the range of exponents found in the literature (from a combination of theoretical modelling and observational works) for AGB CSEs, typically $\alpha \sim 0.5 - 1$ (e.g. De Beck et al. 2010; Maercker et al. 2016; Danilovich et al. 2015, and references therein). There is some indication from recent works that the kinetic temperature distribution is shallower, with

values of α down to ~ 0.4 , for the inner CSE layers ($\sim 5 \times 10^{14} - 3 \times 10^{15}$ cm; De Beck et al. 2012; Lombaert et al. 2016) than for the outer regions, where the steepest temperature variations ($\alpha \sim 1-1.2$) are found ($\geq 10^{16}$ cm; Teyssier et al. 2006). This is indeed in very good agreement with the small value of α found in the inner envelope layers from our analysis. (The hot-to-warm mass vs. T_{rot} trend with a similar value of α is also deduced in our sample of C-rich targets studied in Paper II). We believe that the empirical relation between the hot-to-warm ratio of M_{H_2} and T_{rot} therefore supports that the double- T_{rot} component identified in some of our objects (and possibly also present in more targets for which CO $J_u > 27$ transitions remain undetected), is a natural consequence of the temperature stratification across the inner envelope layers. Detailed non-LTE excitation and radiative transfer of the CO emission including high- J transitions, $J_u \sim 14-40$, are needed for a proper characterization of the temperature structure in the warm inner-wind regions of AGB stars. See Appendix A for a discussion of non-LTE effects on the RD analysis.

7.2. Comparison with other works: $\dot{M}_{\text{THROES}}$ vs. $\dot{M}_{\text{Bibliography}}$

In Fig. 10 we show, for each source, the mass-loss rate estimated in this work for the adopted radius (r_{CO}) against a mean value of gas mass-loss rates found in the bibliography ($\dot{M}_{\text{Bibliography}}$). We assign error bars of a factor 3 to our estimates of the mass-loss rate; this is a common uncertainty value adopted in most

⁴ Although IRAS 17347-3139 does not deviate significantly from the observed hot-to-warm M_{H_2} vs. T_{rot} trend, we excluded this object from the fit because, being a young PNe, it does not necessarily follows the same density and temperature profiles of the AGB CSEs.

Fig. 8. *Top:* relation between $\dot{M}$ and T_{rot} . Single- and double-fit (warm and hot) values, whenever these exist, are connected using dashed lines. *Middle:* relation between $\dot{M}$ and v_{exp} . The distribution approaches a power-law of the type $\dot{M} \propto v_{\text{exp}}^{2.5}$ (dashed line). *Bottom:* integrated flux of the CO $J = 15-14$ line vs. $\dot{M}$ in a logarithmic scale.

molecular line-emission studies (e.g. Maercker et al. 2016). The error bars of $\dot{M}_{\text{Bibliography}}$ represent the low and high ends of the

Fig. 9. Ratio of the mass and rotational temperatures for the hot and warm components, $M_{\text{H}_2}^{\text{hot}}/M_{\text{H}_2}^{\text{warm}}$ vs. $T_{\text{rot}}^{\text{hot}}/T_{\text{rot}}^{\text{warm}}$, for sources with a double- T_{rot} component, namely, the AGB stars NML Tau, π Gru, W Aql, and χ Cyg and the yPN IRAS 17347-3139. The solid line is a fit by a power-law function ($y \sim x^{-1/\alpha}$) to the AGB stars' data – see text in Sect. 7.1. A similar trend is found in our analogue study of the THROES C-rich sample reported in Paper II.

Fig. 10. Comparison of the mass-loss rates from this work and from the literature (Tables D.2 and D.3, respectively). The solid line represents a 1:1 ratio. Target colour and symbol code as in Fig. 1. The big circles are used to locate a few targets with previous $\dot{M}_{\text{Bibliography}}$ estimates obtained from non-LTE excitation and radiative transfer analysis of CO lines, including some of the PACS transitions.

broad range of values found in bibliography after scaling to our d , v_{exp} and χ_{CO} values, and is always ~ 3 or more. For objects with only one value of $\dot{M}$ from the literature, an uncertainty factor of 3 has also been assumed after scaling.

The comparison between our mass-loss rates and those found in the bibliography is in quite good agreement for all the objects, see also Fig. C.2. As already mentioned, we are particularly interested in the comparison of our $\dot{M}$ with those obtained from comprehensive non-LTE excitation and radiative transfer models that make use of some CO rotational lines (normally, $J < 20$) measured with PACS, which exist for a small

sample of objects: for R Cas, NML Tau, TX Cam, R Dor, W Hya and W Aql (Van de Sande et al. 2018; Maercker et al. 2016; Khouri et al. 2014; Danilovich et al. 2014). We find that, also in these cases, discrepancies with our values are always within 50% for all sources except W Hya, demonstrating that the simple and approximate RD approach and the assumptions (e.g. the adopted size of the emitting layers) used in this work yield reasonable first estimate results.

Considering again our sample as a whole, our mass-loss rate estimations of post-AGBs and PNe seem to be systematically lower than those in the literature by a $\sim 20\%$. In principle, this small difference could suggest that the radius of the CO-emitting region is slightly smaller than the value of r_{CO} adopted by us (at least in some objects). As it is shown in Fig. C.2, a fine tuning of r_{CO} can be performed to obtain a perfect match between $\dot{M}_{\text{Bibliography}}$ and our estimates for each individual object. However, we prefer to treat the sources as homogeneously as possible and to be conservative avoiding the use of very small values of r_{CO} , which would result in large opacities ($\tau \gg 1$) and would consequently lead to unreliable opacity corrections.

A similar discrepancy is reported by Danilovich et al. (2015) from a CO-line study (including non-LTE radiative transfer modelling) of AGB CSEs in the SUCCESS programme including CO transitions from $J = 1-0$ to $J = 9-8$, as well as $J = 14-13$ in some targets. Their models give mass-loss rates that are on average 40% lower than those derived from past studies (see their Fig. 7). Danilovich et al. (2015) note that, as already mentioned here, most past studies are based on observations of a small number of low- J CO transitions (with similar excitation conditions, i.e., E_{up}), and conclude that taking a large sample of CO transitions, including high- J lines, properly into account when modelling mass-loss rates, results in lower derived values.

It is important to stress that the mass-loss rates derived in this work represent average values during the period of time when the warm, inner envelope layers were ejected, that is, during the last $<50-100$ years, for AGBs, and the last $\sim 600-2000$ years, for PNe (considering the values of r_{CO} and v_{exp} given in Table D.3). Since the low- J lines commonly used in the previous studies to derive $\dot{M}_{\text{Bibliography}}$ mainly trace the outer envelope layers, the discrepancies observed with respect to past studies could reflect a real time variation of the mass-loss rate in some cases. This is indeed the case of OH 231.8+4.2, where mass-loss rate when the bulk of the nebula was ejected during the last ≈ 1000 yr ($\sim 2 \times 10^{-4} M_{\odot}$, Alcolea et al. 2001) is much larger than the present-day mass-loss rate ($< 2 \times 10^{-5} M_{\odot}$), Sánchez Contreras et al. 2002). The upper limit to the present-day mass-loss rate of OH 231.8+4.2 is indeed in very good agreement with our estimate using high- J CO transitions.

Finally, as a word of caution we note that the mass-loss rates estimated for post-AGB objects and PNs are particularly uncertain as it is not easy to define essential parameters like r_{CO} or v_{exp} for these spatio-kinematically and morphologically complex objects. This makes the comparison with values from past studies subject to larger uncertainties. In spite of this, the agreement is reasonably good for the two post-AGBs and one PN in our sample with values of $\dot{M}$ reported in the literature.

7.3. Mass and mass-loss rate vs. T_{rot}

As shown in Fig. 7, we find a statistically significant anticorrelation between the total mass of the PACS-CO emitting region, M_{H_2} , and the rotational temperature, T_{rot} , derived from our RD analysis. As expected, a similar trend is present between the mass-loss rate, $\dot{M}$, and T_{rot} (Fig. 8).

Prior to this work, Teyssier et al. (2006) and Danilovich et al. (2015) noticed a tentative $\dot{M}$ vs. T_{rot} anticorrelation based on their studies of the intermediate-to-outer regions of the envelopes of AGB and post-AGB stars using submm/mm-wavelength CO transitions. Particularly, Danilovich et al. (2015) reported $\dot{M}$ and T_{kin} at a representative distance of $\approx 10^{16}$ cm (i.e. ~ 100 times the dust condensation radius) for a sample of 53 AGB stars. From their analysis, using self-consistent non-LTE radiative transfer models of the dust continuum emission and the CO emission transitions over a range of excitations (from $J = 1-0$ to $J = 9-8$, and in a few cases, up to $J = 14-13$), Danilovich et al. (2015) found that in general high mass-loss rate objects show relatively low temperatures (see their Fig. 6).

The temperatures of the regions studied by Danilovich et al. (2015), at distances $\sim [1-2] \times 10^{16}$ cm, range between ~ 10 and 80 K to be compared with the larger temperatures, $\sim 200-600$ K, found by us at distances typically a factor ~ 10 smaller in our AGB+OH/IR targets. This indicates that this trend is preserved from the inner envelope layers, traced by $J_{\text{u}} \geq 14$ CO lines, through the outer parts of the CSE, sampled by lower- J transitions.

As discussed by Danilovich et al. (2015), a possible reason for the anticorrelation observed is the more efficient line cooling expected for high mass-loss rate objects (see also Groenewegen 1994, and references therein). In addition to this, we believe that optical depth effects can partially contribute to, and reinforce, the observed anticorrelation. This is because for high mass-loss rate objects, the $\tau_{\text{CO}} \sim 1$ surface layer, which is the deepest region that can be observationally sampled by a given CO line, is located at larger distances from the star where the gas kinetic temperature is lower.

7.4. Mass and mass-loss vs. expansion velocities

In Sect. 6 we already mentioned the presence of evident correlations between M_{H_2} and v_{exp} and between $\dot{M}$ and v_{exp} (Figs. 7 and 8, respectively).

The correlation found between M_{H_2} and v_{exp} is stronger if we consider only the AGB and OH/IR stars in our sample. In AGB and OH/IRs stars, the observed correlation could be telling us about the processes which are responsible for the acceleration of the stellar wind. Since AGB winds are primarily driven by radiation pressure on dust, the most luminous objects (which are also the most massive) will exhibit the largest expansion velocities.

The fact that post-AGB and PNs deviate from the observed trend is probably related with the different mass-loss mechanism (not driven by radiation pressure on dust) in these latest stages (Bujarrabal et al. 2001).

Moreover, the expansion velocities of post-AGBs and PNs do not represent the terminal velocity of the present-day stellar wind but the result from the complex hydrodynamical interaction between the stellar high-velocity winds, that appear beyond the AGB phase, and the slow ambient circumstellar material (expelled in the previous AGB stage).

Based on the above conclusion that, in AGB stars, v_{exp} correlates with M_{H_2} via the stellar luminosity, the trend found between v_{exp} and $\dot{M}$ is not surprising (Fig. 8). In this case, however, the post-AGBs and PNs in our sample do not deviate significantly from the general trend, although, as we mentioned above, the values and interpretation of v_{exp} as well as the $\dot{M}$ derived (under simplifying assumptions) have to be regarded with caution.

The $\dot{M}$ -to- v_{exp} relation has been observed before in other CO line studies in AGB CSEs. For example, Danilovich et al. (2015)

report a correlation between $\dot{M}$ and v_{exp} including stars of different chemical types (O-rich, C-rich and S-stars), which is in very good agreement with our data-points (in spite of the lower- J transitions, $J < 14$, used by these authors). We have fitted a power-law function to the observed distribution (dashed line in Fig. 8-middle panel), the best fit gives an index of about 3 (i.e., $\dot{M} \propto v_{\text{exp}}^{2.5}$) although the uncertainties associated to the fitting are important (2.5 ± 1).

7.5. Other trends

As shown in Sect. 6, we find a clear and expected correlation between the strength of the CO line emission, in particular, of the $J = 15-14$ line ($F_{\text{CO } 15-14}$), with M_{H_2} and $\dot{M}$ (Figs. 7 and 8, respectively). The correlation found by us is in very good agreement with that reported recently by Lombaert et al. (2016) using a number of CO transitions observed with PACS to model the envelopes of a sample of C-rich AGB CSEs with H_2O emission. The dependence with the distance to the sources of $F_{\text{CO } 15-14}$, M_{H_2} and $\dot{M}$ partially explain the observed trend; additionally, the line flux is proportional to the amount of mass in the emitting volume (Eq. (3)), although other factors, such as the opacity and the excitation temperature, have an important influence.

The influence of the excitation temperature in the resulting strength of the CO lines relative to the continuum becomes evident in Fig. 8-bottom panel, where we see a clear correlation between $F_{\text{CO } 15-14}/\text{PACS}_{170}$ and T_{rot} , which are both distance independent parameters. We find that objects with the lowest values of T_{rot} show small line-to-continuum ($F_{\text{CO } 15-14}/\text{PACS}_{170}$) ratios. We have found from this work that post-AGBs and PNs have the most massive envelopes in our sample ($>0.01-0.1 M_{\odot}$), but in spite of this, they are relatively weak high- J CO emitters as a consequence of the relatively low excitation conditions prevailing in their envelopes ($T_{\text{rot}} \sim 200-300$ K). Other factors, such as a different gas-to-dust mass fraction at different evolutionary stages, may also lie behind the observed trend.

8. Summary

We have analysed *Herschel*-PACS 1D spectra of 26 evolved low-to-intermediate mass stars, in different evolutionary stages from the AGB to the PN phase, contained in the THROES catalogue⁵. Our sample includes 23 O-rich and 3 S-type objects (C-rich targets are separately studied in Paper II).

RDs using high-excitation CO $v = 0$ rotational emission lines, with upper-level energies $E_{\text{up}} \sim 580-5000$ K, have been created to study the warm inner layers of the CSEs of these objects. We derive fundamental physical parameters such as: rotational temperatures (T_{rot}), total molecular mass in the CO-emitting layers (M_{H_2}) and average mass-loss rates during the ejection of these layers ($\dot{M}$).

The rotational temperatures are found to vary from ~ 200 K to ~ 700 K. For AGB and OH/IR stars, which represent $\sim 80\%$ of our sample, the rotational temperatures are around $T_{\text{rot}} \sim 500$ K and systematically larger than for the most evolved objects, post-AGBs and PNs ($T_{\text{rot}} \sim 200$ K). These temperatures are one order of magnitude higher than estimated from past low- J CO line studies of the outer envelope. This is expected as, in the PACS far-infrared range, we are tracing gas that is closer to the central star ($\approx 10^{15}$ cm for AGBs and $\approx 10^{16}$ cm for post-AGBs and PNs).

The total mass of the inner CSE regions where the PACS CO lines arise ranges from $M_{\text{H}_2} \sim 10^{-6}$ to $10^{-2} M_{\odot}$ in our sam-

ple, with the most evolved objects being the most massive. The values of M_{H_2} found in this work are typically 100–1000 times lower than the total envelope mass obtained from previous low- J CO line studies.

The mass-loss rates estimated are in the range $\dot{M} \approx 10^{-7}-10^{-4} M_{\odot} \text{ yr}^{-1}$, in agreement (within uncertainties) with values found in the literature.

For some strong CO emitters in our sample (NML Tau, χ Cyg, W Aql, NML Cyg and IRAS 17347–3139) a double temperature (hot and warm) component is inferred. The temperatures of the warm and hot components are $\sim 400-500$ K and $\sim 600-900$ K, respectively. The mass of the warm component ($\sim 10^{-5} - 8 \times 10^{-2} M_{\odot}$) is always larger than that of the hot component, by a factor $\sim 2-10$.

The warm-to-hot M_{H_2} and T_{rot} ratios in our sample are correlated and are consistent with an average temperature radial profile of $\propto r^{-0.5 \pm 0.1}$, that is, slightly shallower than in the outer envelope layers, in agreement with recent studies.

We have explored the distributions of the different magnitudes and physical parameters of these objects and if any trends exist. We find that M_{H_2} and $\dot{M}$ are both anticorrelated with T_{rot} . This is interpreted as a combination of two different processes: CO line cooling and opacity effects. Previous works have also reported similar trends based on low- J CO line observations.

A strong correlation has been found, also, between M_{H_2} and v_{exp} , particularly for AGB stars. This correlation is also present in the $\dot{M}$ vs. v_{exp} distribution, as expected. This trend, which is observed in past studies using low- J CO transitions, is consistent with the wind acceleration mechanism being more efficient in the more luminous and massive stars.

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⁵ <https://throes.cab.inta-csic.es>

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Appendix A: Non-LTE effects

The rotational diagram (RD) method is a classical and widely used line-emission analysis technique useful to obtain a first estimate of the excitation temperature and mass of the gas in the line emitting region (Goldsmith & Langer 1999; Justtanont et al. 2000). As explained in Sect. 5, it is based on two major assumptions: optically thin emission and excitation under LTE conditions. A canonical opacity correction factor, C_τ , has been included to take into account moderate optical depth effects (Sect. 5). Here, we examine whether non-LTE excitation effects are expected to be significant in our sample and, if this is the case, what is the impact on the values of M_{H_2} and T_{rot} inferred from our RD analysis. We present several arguments that suggest that although small LTE deviations cannot be ruled out (particularly, in the lowest mass-loss rate objects), we expect a negligible impact on the derived values of M_{H_2} . Additionally, the double slope in the RD observed for some targets predominantly reflects the temperature stratification in the emitting layers.

A first simple evaluation of LTE deviations is obtained from the comparison of the critical densities of the CO transitions studied here and the densities expected in the CO-emitting regions in our sample. For most (80%) of our targets, the far-IR CO transitions detected and used in our RD analysis arise from states ~ 500 – 2000 K above the ground, i.e. with upper-level rotational quantum numbers $J_u \sim 14$ – 27 . According to most recent collisional rate coefficients computed by Yang et al. (2010)⁶, these transitions have critical densities of $n_{\text{crit}} \sim 5 \times 10^5$ and $3 \times 10^6 \text{ cm}^{-3}$, for $J_u = 14$ and $J_u = 27$, respectively, for a range of temperatures consistent with our estimates, ~ 200 and 700 K, see Fig. 10 in Yang et al. (2010).

From the lowest to the highest mass-loss rate objects in our sample ($\dot{M} \sim 2 \times 10^{-7}$ – $1 \times 10^{-4} M_\odot \text{ yr}^{-1}$, Fig. 8), densities of $n_{\text{H}_2} \gtrsim 10^6$ – 10^8 cm^{-3} are expected at the typical radius adopted (from $r_{\text{CO}} \sim 4 \times 10^{14}$ to $r_{\text{CO}} \sim [1\text{--}4] \times 10^{15} \text{ cm}$, respectively – see Table D.2, Appendix B) consistent with CO population levels predominantly thermalized in most cases.

As already pointed out in pioneering studies of ISO-LWS observations of high- J CO lines using the RD approach, see Justtanont et al. 2000, the mere fact that we detect CO $J_u \sim 14$ – 27 transitions together with a roughly linear distribution in the RD is a hint of high-density gas and level populations in this range of J_u close to thermal equilibrium.

For a few targets, we also detect CO lines with upper-levels above $J_u > 27$, which have critical densities of $n_{\text{crit}} \sim 10^6$ – 10^7 cm^{-3} and, therefore, some LTE deviations cannot be ruled out (but we note that these transitions presumably arise from regions closer to the center, within the dust formation layers).

The simple calculations above are indeed corroborated by non-LTE excitation and radiative transfer analysis computations of a selection of high- J CO transitions observed with PACS (from $J_u = 14$ to 38) on a sample of C-rich AGB CSEs by Lombaert et al. (2016). These authors conclude that over the broad range of mass-loss rates studied in their work, $\dot{M} \sim 10^{-7}$ – $2 \times 10^{-5} M_\odot \text{ yr}^{-1}$, which is comparable to the range in our sample, the CO molecule is predominantly excited through collisions with H_2 , with a minor effect of far-IR radiative pumping due to the dust radiation field.

We stress that even under non-LTE conditions, for a simple diatomic molecule like CO, the RD method provides a reliable measure of the total mass within the emitting volume. This is because, although T_{rot} may deviate from the kinetic temperature, T_{kin} , in regions where the local density is lower

than the critical densities of the transitions considered, it does describe quite precisely the molecular excitation (i.e. the real level population). To test this idea and to check the reliability of our analysis, we have compared our values of M_{H_2} and $\dot{M}$ with those obtained from state-of-the-art line excitation and radiative transfer models of high- J CO transitions, sometimes including PACS data, performed by other authors in objects of our sample. To our knowledge, these have been published for a total of 6 sources: R Cas, R Dor, TX Cam, NML Tau, W Hya and W Aql (see Van de Sande et al. 2018; Maercker et al. 2016; Danilovich et al. 2014; Khouri et al. 2014 and references therein). For these objects, the CO emission over a broad range of E_{up} has been modelled to derive the temperature, density and velocity profile across their $\sim 10^{14}$ – 10^{17} cm CSE layers, as well as the mass-loss rate of the stellar wind. As shown in Sect. 6, discrepancies between our values of $\dot{M}$ and those obtained from comprehensive non-LTE radiative transfer analysis are very small, always within 50%, demonstrating that the simple and approximate RD approach and the assumptions (e.g. the adopted size of the emitting layers) used in this work yield reasonable results.

An additional test of the reliability and uncertainties of the RD method is presented in Paper II, where we perform our RD analysis using multi-epoch CO-PACS spectra for the C-rich AGB star IRC+10216. This object shows prominent line variability (mainly of high-excitation transitions of CO and other molecules) denoting radiative farIR (ro-vibrational) pumping via the dust radiation field modulated by the stellar pulsation (Cernicharo et al. 2014; Teyssier et al. 2015; He et al. 2017). This object, thus, serves as a benchmark for testing the effect of radiative vs. collisional excitation and its impact of the values of M_{H_2} and T_{rot} derived from our RD analysis. We corroborate that, in spite of strong CO line flux variations and confirmed changes in the relative level population, the total number of emitting molecules (adding up all levels) from the RD analysis remains constant (within uncertainties, $< 15\%$) at multiple epochs. This is true for both the warm and hot components (both identified in IRC+10216) and, thus, for the single-fit value of M_{H_2} .

We also find that line variability has also a small impact on the value of T_{rot} derived at multiple epochs in IRC+10216. The values of T_{rot} from the single-fit and warm component (using $J_u < 27$ transitions) remain essentially constant within uncertainties, consistent with negligible impact of non-LTE effects (if any). The highest-excitation CO lines ($J_u > 27$) show stronger variations and, as a consequence, the variations of T_{rot} for the hot component are larger, of $\lesssim \pm 15\%$ about the average, maybe denoting some repercussion of LTE deviations on T_{rot} in this case.

Although it is improbable given our previous discussion, let us now consider whether the double slope in the RD diagram found for a few objects in our sample could predominantly result from non-LTE effects, with T_{rot} deviating most significantly from T_{kin} for the highest- J CO transitions, and what would be the implications in this case.

Among our targets (O-rich and S-type), we find a double- T_{rot} component in a total of five sources, covering a broad range of mass-loss rates, from $\dot{M} \sim 2 \times 10^{-7}$ to $8 \times 10^{-5} M_\odot \text{ yr}^{-1}$. The mass-loss rate distribution of these sources is the same as the sources for which only one T_{rot} component is found. Moreover, we do not find any correlation between $\dot{M}$ and the properties of the hot and warm components (also including C-rich targets, see e.g. Fig. A.1), which makes improbable the double T_{rot} component being predominantly a non-LTE effect (expected to be most remarkable in low mass-loss rate objects).

⁶ Also available from the Leiden Lambda Database web page.

Fig. A.1. Ratio of the hot-to-warm rotational temperature vs. the mass-loss rates for objects with a double- T_{rot} component: targets from this work (Paper I) are represented by open symbols, C-rich objects (from Paper II) are plotted using filled symbols.

Moreover, to explain the observed double slope as a purely non-LTE effect, two conditions need to be simultaneously met in all double- T_{rot} targets. First, a very specific value of the number density, in a narrow range around $\sim 10^7 \text{ cm}^{-3}$, is needed to have $J_u < 27$ levels close to thermal equilibrium but $J_u > 27$ levels deviating perceptibly from LTE (this would generate the double slope in the RD diagram). Second, a strong background radiation source $T_{\text{bg}} > T_{\text{kin}}$ is required to reproduce a T_{rot} that is higher for $J_u > 27$ transitions than for $J_u < 27$ lines. Dust mixed with the gas in the CO-emitting volume and heated by the stellar radiation to 800 K could produce the required T_{bg} . If this is the case, then it would also imply similarly high gas temperatures in the emitting region since the difference between the gas and dust temperature across these inner wind layers is expected to be moderate (of $< 100 \text{ K}$) and to follow a similar radial dependence based on detailed dust-continuum and non-LTE radiative transfer CO emission models (e.g. for W Aql, $T_{\text{kin}} \sim T_{\text{dust}} \sim 300 \text{ K}$ at $r_{\text{CO}} = 2 \times 10^{15} \text{ cm}$ Danilovich et al. 2014). In the extreme case (e.g. maybe for very low mass-loss rate objects with densities $< 10^6 \text{ cm}^{-3}$) that T_{rot} is totally decoupled from T_{kin} but very close to T_{bg} for all transitions from $J_u = 14$ to 40, then the double-slope of the RDs would most likely reflect the stratification of the dust temperature (rather than the gas) across the envelopes.

Summarizing, a minor impact of small LTE deviations on the values of M_{H_2} and $\dot{M}$ is expected, even for the targets with the lowest mass-loss rates, $\dot{M} \approx 10^{-7} M_{\odot} \text{ yr}^{-1}$. The double slope of the RD is unlikely to be primarily due to large LTE deviations and points to a temperature stratification in the warm inner layers of the envelopes probed by PACS CO line emission. The temperature profile deduced is further discussed in Sect. 7.1.

Appendix B: The characteristic radius of the CO-emitting volume

In this appendix, we provide a more detailed description of the procedure that we have followed to decide on a “characteristic” radius of the CO-emitting volume (r_{CO}) to be used to compute,

Fig. B.1. Power-law radial distribution of the gas kinetic temperature estimated from non-LTE excitation and radiative transfer models of the CO emission in a number of AGB envelopes (indicated at the top of the box using the same colour for the temperature laws) from the literature. References: Van de Sande et al. (2018), Maercker et al. (2016), Khouri et al. (2014), Decin et al. (2010). The solid and dotted lines of R Dor and IK Tau are different temperature profiles derived by different authors (solid from Maercker et al. 2016, and dotted from Van de Sande et al. 2018 – R Dor and Decin et al. 2010 – IK Tau). The thick black line is an average temperature law.

and correct for, the CO line opacities (Sect. 5.1) and to obtain an estimate of the mean mass-loss rate of our targets (Sect. 6.2).

For AGB CSEs (also including OH/IRs), a first estimate of the size of the CO-emitting volume is derived using the envelope temperature structure estimated from detailed non-LTE excitation and radiative transfer calculations in the literature. These exist for many AGB CSEs using low- J CO transitions (typically $J_u \leq 6$), and, for more reduced samples, also using certain CO transitions from higher J levels.

In Fig. B.1 we show temperature power-law radial profiles in the form

$$T(r) = T_i \times \left(\frac{r}{R_i}\right)^\alpha$$

that have been deduced in a number of previous works (references are given in the figure caption) for the few targets in our sample that include at least one high- J CO line observed with any of the three *Herschel* instruments (HIFI, SPIRE, or PACS). As we see in this figure, the full range of rotation temperatures deduced from our RD analysis, $T_{\text{rot}} \sim 200\text{--}700 \text{ K}$ (Sect. 6), is consistent with the bulk of the PACS CO emission studied here arising from layers between $\sim 2 \times 10^{14}$ and $\sim 5 \times 10^{15} \text{ cm}$, if we take together all the $T(r)$ distributions in Fig. B.1 (coloured lines), or between $\sim 3 \times 10^{14}$ and $\sim 3 \times 10^{15} \text{ cm}$, if we use an average $T(r)$ power-law (thick black line, in Fig. B.1). The quadratic mean of these two ranges is $r_{\text{CO}} \sim 10^{15} \text{ cm}$, which we uniformly use as the reference value in most AGB stars to compute M_{H_2} , T_{rot} , and $\dot{M}$ (but see more details below). Since the radius is, in any case, uncertain, we offer additional estimates of these parameters for a larger range of radius around the default r_{CO} (Appendix C). As we will see next, for the lowest (larger) mass-loss rate AGB stars in our sample, the characteristic CO-radius could be a factor of $\sim 2\text{--}4$ smaller (larger) than the $r_{\text{CO}} \sim 10^{15} \text{ cm}$ reference value.

In the following, we perform a case-by-case RD analysis of three targets (R Dor, W Aql, and TX Cam) that are representative of three main mass-loss regimes in our sample: low, medium

and high ($\dot{M} \approx 10^{-7} M_{\odot} \text{ yr}^{-1}$, $\approx 10^{-6} M_{\odot} \text{ yr}^{-1}$, and $\geq 10^{-5} M_{\odot} \text{ yr}^{-1}$, respectively) and for which detailed non-LTE excitation and radiative transfer studies of the CO emission including some mid-to-high J_u -CO transitions exist in the literature. The purpose is twofold: (1) to better illustrate our method to constrain r_{CO} in our sample (needed to decide on a plausible reference value for a uniform analysis), and (2) to compare the mass-loss rates from our approximate RD analysis with those computed using more sophisticated modelling tools.

R Dor. Precise CO-modelling studies of the molecular envelope of this object, including CO transitions up to $J_u = 16$ ($E_{\text{up}} = 750 \text{ K}$), have been carried out by Maercker et al. (2016) and Van de Sande et al. (2018; references to other molecular line studies using lower- J_u transitions are given in Table D.2). The gas temperature structure deduced from these works, which use the same set of CO lines, are not fully coincident (dotted and solid red lines in Fig. B.1). Van de Sande et al. (2018) claim that their model achieves a better fit to more lines, and therefore, we adopt the $T(r)$ power-law determined by these authors, with an exponent $\alpha = 0.65$.

Our general procedure to determine an optimal/acceptable value of r_{CO} is as follows. From a linear fit to the CO datapoints in the RD diagram (dotted line and black dots, respectively, in the top panel of Fig. B.2) we find a first or iteration-zero estimate of $T_{\text{rot}}(i = 0)$ before any opacity correction is applied. Assuming that $T_{\text{rot}}(i = 0) \sim 570 \text{ K}$ represents (or is close to) the average gas temperature within the CO-emitting volume and using the $T(r)$ function depicted in Fig. B.1, we derive an initial value of $r_{\text{CO}}(i = 0) \sim 2.5 \times 10^{14} \text{ cm}$. We use this radius to compute the opacity of the different transitions. In this case, we obtain $\tau_{14 \rightarrow 13} \sim 1.8$ for the CO $J = 14-13$ line, and smaller for higher- J lines (see Eq. (4)). After applying the opacity correction, through the frequency-dependent factor $C_{\tau} = \tau/(1-e^{-\tau})$, a second linear fit to the opacity-corrected datapoints is performed (pink line and dots, respectively, in top panel of Fig. B.2), resulting in a new estimate of $T_{\text{rot}}(i = 1)$. The latter always is smaller than the iteration-zero value because after applying the C_{τ} correction, the slope of the RD increases, as a direct result of the frequency-dependence of C_{τ} and the typical values of T_{rot} that we measure in our sample. Comparing again the value of $T_{\text{rot}}(i = 1) \sim 480 \text{ K}$ with the $T(r)$ law, we deduce a new value of $r_{\text{CO}}(i = 1) \sim 3.4 \times 10^{14} \text{ cm}$, where the gas would have such a temperature.

This exercise indicates that an intermediate value between $r_{\text{CO}}(i = 0)$ and $r_{\text{CO}}(i = 1)$ is needed to reach full consistency between the r_{CO} value used for the opacity correction and the one that reproduces the opacity-corrected T_{rot} derived (according to the $T(r)$ adopted). In the particular case of R Dor, we find a perfect match between $r_{\text{CO}}(i = 0)$ and $r_{\text{CO}}(i = 1)$ for $r_{\text{CO}} \sim 3.15 \times 10^{14} \text{ cm}$ (leading to $T_{\text{rot}}(i = 1) \sim 500 \text{ K}$ at this radius – Fig. B.1, middle panel).

An additional constrain to the radius is obtained from the fact that, as already explained in Sect. 5, the deepest layer traced by the observed CO emission must be such that $\tau < 1$. In order to satisfy this moderate-opacity condition, a value of r_{CO} slightly larger than the “perfect-match” r_{CO} above is preferred. For R Dor, a value of $r_{\text{CO}} \sim 3.5 \times 10^{14} \text{ cm}$ satisfies the opacity criteria ($\tau_{14 \rightarrow 13} < 1$) and is, within uncertainties, still fully consistent with the radius where the final value of T_{rot} is attained, adopting the $T(r)$ law from previous works – Fig. B.2, bottom panel). The mass-loss rate that results adopting this value of the radius $r_{\text{CO}} \sim 3.5 \times 10^{14} \text{ cm}$, which guarantees line opacities lower than 1, is $\dot{M} \sim 4 \times 10^{-7} M_{\odot} \text{ yr}^{-1}$.

In this and in most targets, in principle we cannot rule out a larger radius (leading to even lower line opacities), even if

Fig. B.2. Rotational diagrams of the low mass-loss rate O-rich AGB star R Dor to illustrate the different steps that we have routinely followed to constrain r_{CO} in our sample. The *bottom panel* shows an optimal value of r_{CO} according to our temperature-opacity combined criteria (full details are given in the text, Appendix B).

Fig. B.3. Rotational diagram of W Aql and NML Tau (*bottom*). *Left*: results of the RD for $r_{\text{CO}} = 1 \times 10^{15}$ cm, which results in a perfect match between the opacity- and temperature-radius (labelled as r_{CO} and r_T , respectively, in the plot) but results in an undesired large opacity correction, $\tau_{14 \rightarrow 13} > 1$. *Right*: results of the RD for $r_{\text{CO}} = 1.4 \times 10^{15}$ cm, which satisfies our $\tau_{14 \rightarrow 13} < 1$ criteria.

T_{rot} deviates from the gas temperature predicted at that radius based on the $T(r)$ law adopted. This is because there is no guarantee that the adopted $T(r)$ is a 100% accurate representation of the real temperature structure in these inner-wind regions and because T_{rot} may not be either a 100% accurate representation of the temperature of the gas (especially for low mass-loss rate objects). For R Dor, if we adopt the default radius of $r_{\text{CO}} \sim 1 \times 10^{15}$ cm previously established as a reasonable characteristic radius for the overall AGB class, we deduce a temperature of $T_{\text{rot}} \sim 570$ K and a mass-loss rate of $\dot{M} \sim 1 \times 10^{-7} M_{\odot} \text{ yr}^{-1}$.

For R Dor, the mass-loss rates derived from Van de Sande et al. (2018) and Maercker et al. (2016) from their non-LTE CO excitation and radiative transfer analysis are very similar in both cases ($\sim 2 \times 10^{-7} M_{\odot} \text{ yr}^{-1}$) and lie within the range of values estimated by us from our simple RD approach and the plausible range of r_{CO} explored, $\dot{M} \sim [1-4] \times 10^{-7} M_{\odot} \text{ yr}^{-1}$.

W Aql. Non-LTE excitation and radiative transfer of the CO emission, including CO transitions up to $J_u = 25$ ($E_{\text{up}} = 1796$ K), have been carried out for this S-type AGB star by Danilovich et al. (2014). The mass-loss rate obtained in this work is $\dot{M} \sim 4 \times 10^{-6} M_{\odot} \text{ yr}^{-1}$ (as quoted in Table D.2, where we provide additional references to other molecular line studies using lower- J_u transitions). Danilovich et al. (2014) derive the gas and dust temperature profile in the 2×10^{14} – 10^{17} cm envelope layers (see their Fig. 3). Both the gas and dust temperatures are quite similar throughout the whole envelope, with the dust being slightly cooler than the gas below 2×10^{15} cm (i.e. the region sampled by the PACS CO data). In this region, the gas and dust temperatures do not differ by more than 50% (in particular, at $\sim 10^{15}$ cm, values of $T_{\text{dust}} \sim 400$ K and $T_{\text{kin}} \sim 500$ K are expected).

In Fig. B.1 we reproduce the gas temperature structure deduced by Danilovich et al. (2014); the exponent of this power-law function is $\alpha = 0.65$. We have used this profile

to constrain r_{CO} following the same procedure explained in the previous paragraphs for R Dor. As we can see in the left panel of Fig. B.3, a radius of $r_{\text{CO}} \sim 1 \times 10^{15}$ cm produces a perfect match between the final (opacity-corrected) temperature derived ($T_{\text{rot}} \sim 500$ K) and the radius where this temperature is expected (r_T) according to Danilovich et al. (2014). This value of the radius, however, results in line opacities larger than desirable and a mass-loss rate of $\dot{M} \sim 9 \times 10^{-6} M_{\odot} \text{ yr}^{-1}$. In this case, the radius that produces $\tau_{14 \rightarrow 13} < 1$ and simultaneously satisfies (within uncertainties) the temperature criteria is $r_{\text{CO}} \sim 1.4 \times 10^{15}$ cm (right panel of Fig. B.3). This results in a somewhat smaller mass-loss rate of $\dot{M} \sim 5 \times 10^{-6} M_{\odot} \text{ yr}^{-1}$, which is in excellent agreement with previous estimates.

IK Tau. The physical properties of the circumstellar gas, including the temperature, velocity and density structure, have been determined from the radiative transfer modelling of the multi-transitional (sub)millimetre CO line observations by Decin et al. (2010) and Maercker et al. (2016). The temperature distributions from these two works differ substantially (as for R Dor) and are shown in Fig. B.1 (solid and dotted cyan lines).

Adopting the $\alpha = 0.6$ distribution derived by Decin et al. (2010), we find that a radius of $r_{\text{CO}} \sim 5 \times 10^{14}$ cm produces a perfect match between the final (opacity-corrected) value of the temperature ($T_{\text{rot}} = 420$ K) and the radius r_T where this temperature is expected, however, it results in opaque lines (Fig. B.3, bottom-left). For IK Tau, a radius of $r_{\text{CO}} \sim 9 \times 10^{14}$ cm or larger is needed to meet the $\tau_{14 \rightarrow 13} < 1$ criteria (Fig. B.3, bottom-right). This results in a somewhat smaller mass-loss rate of $\dot{M} \sim 1 \times 10^{-5} M_{\odot} \text{ yr}^{-1}$, also in agreement with the range of values from previous estimates ($\dot{M} \sim [0.2-3.5] \times 10^{-5} M_{\odot} \text{ yr}^{-1}$, Table D.2).

Rest of the targets. We have followed this procedure to constrain the range of r_{CO} values that are plausible (based on our opacity- and temperature- combined criteria) for each target individually. Whenever a $T(r)$ distribution was available in the literature (this happened for a few targets, see Fig. B.1) we used that specific law, and for the rest we used a mean $T(r)$ distribution represented by the thick black line in Fig. B.1 as a guide.

Remarks on the temperature profiles. The $T(r)$ profiles used and represented in Fig. B.1, although obtained from detailed non-LTE excitation and radiative transfer models of the CO emission, are not free from large uncertainties. This is denoted by the discrepancies between the temperature structure derived for the same targets when computed by different teams (notable cases are R Dor and IK Tau, in spite of these being among the most studied and best characterized AGB envelopes). Moreover, the power-law distribution is only an approximation to the real temperature structure. Indeed, the latter can deviate significantly from a simple power-law in some regions, in particular, $T(r)$ can have multiple-slopes as well as local minima and maxima as shown in De Beck et al. (2010, see their Fig. 9) and Maercker et al. (2016, see their Fig. 5).

Additionally, given the moderate range of J_u in the CO transitions predominantly modelled and published to date, the curves represented in Fig. B.1 are expected to be most reliable in the intermediate-to-outer envelope layers, beyond $\sim 10^{15}$ cm. Recently, Lombaert et al. (2016) performed non-LTE excitation and radiative transfer models of a sample of C-rich AGB CSEs

using a selection of seven high- J CO transitions observed with PACS and SPIRE covering levels from $J_u = 15$ to 38, that is, higher than in the studies represented in Fig. B.1. One interesting result from this study is that the temperature of the gas falls off less steeply, with a power-law exponent close to $\alpha \sim 0.4-0.5$, in the inner-warm envelope regions sampled by these high- J CO transitions. This is indeed consistent with the crude estimate of α deduced in this work by comparing the hot and warm envelope components for a few targets in our sample (see Sect. 7). More dedicated non-LTE excitation and radiative transfer models of the high- J CO emission in larger samples is needed to confirm this result and to obtain a more precise description of the temperature distribution in these inner and warm regions of the envelopes of AGB stars.

Final remark on the reference values of r_{CO} . It is evident that the value of r_{CO} derived using a temperature criteria is very model-dependent since it fully relies on $T(r)$ and on T_{rot} being a perfect representation of T_{kin} . For this reason, we prefer to be cautious and, after having explored carefully the range of plausible r_{CO} values based on a temperature-opacity combined criteria for all targets, to use a set of (order-of-magnitude) estimates of r_{CO} for the whole sample, rather than using the best-match radius individually found for each target. As shown in Table D.2, we chose a reference radius: $r_{\text{CO}} = 1 \times 10^{15}$ cm for most AGB CSEs, $r_{\text{CO}} = [2-4] \times 10^{15}$ cm for high- $\dot{M}$ AGB CSEs ($> 1 \times 10^{-5} M_{\odot} \text{ yr}^{-1}$) and $r_{\text{CO}} = [4-6] \times 10^{14}$ cm for low- $\dot{M}$ AGB CSEs ($< 1 \times 10^{-6} M_{\odot} \text{ yr}^{-1}$).

As discussed in Sect. 5, the temperature profile in the molecular envelopes of post-AGB objects and PN is extremely poorly characterized due to a much more limited number of CO emission cartography and, most importantly, modelling studies (especially using high- J CO transitions). Based on the systematically low values of T_{rot} in post-AGB objects and PNs found in this work (~ 200 K) as well as their generally larger dimensions, we chose a reference value of the radius of $r_{\text{CO}} = 6 \times 10^{16}$ cm in these cases (Table D.3), although we explored a larger range of r_{CO} (examples are given in Figs. C.1 and C.2). This range of r_{CO} resulted in negligible RD opacity corrections in all these sources.

Appendix C: Additional opacity and mass-loss rate plots

In this appendix we show, for each source, the values of the optical depth (τ , defined in Sect. 5.1) of the different CO transitions used to build the RDs for a range of values of the characteristic radius (r_{CO}) of the CO-emitting volume (Fig. C.1). As we can see in this figure, the radius adopted implies a moderate value of τ and, therefore, a moderate opacity correction. The radius of the PACS CO-emitting region is the major source of uncertainty in the computation of τ and, therefore, of the emitting mass and mass-loss rates. It also has an effect on the rotational temperature. The values of M_{H_2} and T_{rot} for a range of r_{CO} are plotted inside the boxes in Fig. C.1. The resulting mass-loss rates, $\dot{M}$, are shown in Fig. C.2, together with the broad range of mass-loss rates found in the literature for each object, typically derived from low- J CO line studies (references are provided in Table D.2).

Fig. C.1. Plots of τ vs. E_{up} corresponding to different linear radii. In each chart there is a subgraphic showing M_{H_2} vs. T_{rot} . The thickest curve and the biggest point are those associated to the r_{CO} shown in Table D.3.

Fig. C.1. continued.

Fig. C.1. continued.

Fig. C.2. Plots of $\dot{M}$ vs. T_{rot} . In each panel three different points, corresponding to three different r_{CO} are shown. The point of the r_{CO} shown in Table D.3 is bigger than the rest. The grey region represents the interval of mass-loss rates covered by previous works found in bibliography. For more details see Sect. 6. The linear radii explored are the same as the ones shown in Fig. C.1.

Fig. C.2. continued.

Appendix D: Tables

Table D.1. Observations log.

Target name	Alternative name	Class	RA (J2000) (hh:mm:ss.s)	Dec (J2000) (dd:mm:ss.s)	Obs IDs	Observing date (yyyy-mm-dd)
RR Aql	–	O-rich AGB	19:57:36.1	–1:53:11.3	1342269414	2013-04-05
Omi Cet	Mira	O-rich AGB	2:19:20.8	–2:58:39.5	1342213286	2011-01-25
					1342213286	2011-01-25
W Hya	–	O-rich AGB	13:49:02.0	–28:22:03.5	1342212604	2011-01-14
					1342223808	2011-07-09
IRAS 20038-2722	V1943 Sgr	O-rich AGB	20:06:55.2	–27:13:29.8	1342268730	2013-03-29
					1342268569	2013-03-27
T Cep	–	O-rich AGB	21:09:31.8	68:29:27.2	1342246557	2012-06-01
					1342203679	2010-08-28
NML Tau	IK Tau	O-rich AGB	3:53:28.8	11:24:22.6	1342203680	2010-08-28
					1342203681	2010-08-28
R Dor	–	O-rich AGB	4:36:45.6	–62:04:37.8	1342197794	2010-06-05
					1342197794	2010-06-05
TX Cam	–	O-rich AGB	5:00:50.4	56:10:52.6	1342225855	2011-08-08
					1342225856	2011-08-08
X Her	–	O-rich AGB	16:02:39.2	47:14:25.3	1342197802	2010-06-05
					1342202120	2010-07-28
IRAS 19474-0744	GY Aql	O-rich AGB	19:50:06.3	–7:36:52.5	1342268638	2013-03-25
					1342268449	2013-03-26
					1342268729	2013-03-29
T Mic	–	O-rich AGB	20:27:55.2	–28:15:39.8	1342268788	2013-03-29
					1342269458	2013-04-06
R Cas	–	O-rich AGB	23:58:24.9	51:23:19.7	1342212576	2011-01-12
					1342212577	2011-01-12
EP Aqr	–	O-rich AGB	21:46:31.9	–2:12:45.9	1342270639	2013-04-20
					1342270684	2013-04-21
NML Cyg	–	O-rich AGB	20:46:25.5	40:06:59.6	1342198174	2010-06-02
					1342198174	2010-06-02
χ Cyg	–	S-type	19:50:33.9	32:54:50.6	1342198176	2010-06-02
					1342198177	2010-06-02
π Gru	–	S-type	22:22:44.2	–45:56:52.6	1342210397	2010-11-28
					1342210398	2010-11-28
W Aql	–	S-type	19:15:23.4	–7:02:49.9	1342209731	2010-11-06
					1342209732	2010-11-07
WX Psc	IRC +10011	OH/IR star	1:06:26.0	12:35:53.0	1342202121	2010-07-28
					1342202122	2010-07-28
V1300 Aql	IRC -10529	OH/IR star	20:10:27.9	–6:16:13.6	1342269516	2013-04-07
					1342269910	2013-04-11
OH 231.8+4.2	–	OH/IR star	7:42:16.8	–14:42:52.1	1342196694	2010-05-19
					1342196695	2010-05-19
OH 26.5+0.6	V437 Sct	OH/IR star	18:37:32.5	–5:23:59.4	1342207776	2010-10-31
					1342207777	2010-10-31
IRAS 22036+5306	–	O-rich p-AGB	22:05:30.3	53:21:33.0	1342221882	2011-05-29
					1342221883	2011-05-29
AFGL 6815	Cotton Candy Nebula	O-rich p-AGB	17:18:19.9	–32:27:20.2	1342216629	2011-03-22
					1342216630	2011-03-22
IRAS 17347-3139	–	O-rich PN	17:38:01.3	–31:40:58.0	1342229696	2011-09-24
					1342229697	2011-09-24
NGC 6537	Red Spider Nebula	O-rich PN	18:05:13.1	–19:50:34.9	1342231322	2011-10-22
					1342231323	2011-10-22
NGC 6302	Butterfly Nebula	O-rich PN	17:13:44.2	–37:06:15.9	1342230150	2011-10-05
					1342230151	2011-10-05

Table D.2. Stellar and circumstellar information taken from the bibliography for the objects of the sample.

Target name	Variability	T_{eff} (K)	d (pc)	v_{exp} (km s ⁻¹)	$\dot{M}_{\text{Bibliography}}$ ($M_{\odot}$ yr ⁻¹)	References
RR Aql	Mira	2000	530	9.0	2.4×10^{-6} 9.1×10^{-7} (0.9,6.2) $\times 10^{-6}$	7, 34
Omi Cet	Mira	2200	110	8.1	2.5×10^{-7} 5×10^{-7} (0.2,1.2) $\times 10^{-6}$	18, 29, 34
W Hya	SRa	2200	98	7.0	1.5×10^{-7} 7.8×10^{-8} 10^{-7} (0.3,3.8) $\times 10^{-7}$ 7×10^{-8} 8.1×10^{-8}	10, 12, 18, 23, 32, 34
IRAS 20038-2722	SRb	2200	197	5.4	9.9×10^{-8} 1.3×10^{-7} (0.7,3.9) $\times 10^{-7}$	7, 14, 32
T Cep	Mira	2400	190	5.5	9.1×10^{-8} (0.8,2.4) $\times 10^{-7}$	7
NML Tau	Mira	2700	260	19.0	5×10^{-6} 8×10^{-6} 2×10^{-5} 4.5×10^{-6} (0.2,3.5) $\times 10^{-5}$ 10^{-5} 4.7×10^{-6} 4.4×10^{-6}	3, 10, 18, 19, 23, 27, 34
R Dor	SRb	2800	59	5.7	1.6×10^{-7} 2×10^{-7} 1.3×10^{-7} (0.9,4.2) $\times 10^{-7}$ 6.9×10^{-8}	1, 3, 10, 23, 32, 34
TX Cam	Mira	2800	380	18.5	4×10^{-6} 5.5×10^{-6} 7×10^{-6} (0.2,1.5) $\times 10^{-5}$ 6.5×10^{-6}	3, 10, 18, 23, 24
X Her	SRV	2800	137	6.5	1.5×10^{-7} 10^{-6} (0.8,2.6) $\times 10^{-7}$	14, 32, 34
IRAS 19474-0744	SR	2800	810 ^a	13.6	4.1×10^{-6} (0.5,1.6) $\times 10^{-5}$	34, 35
T Mic	SRb	2800	290	4.8	8×10^{-8} 2.7×10^{-7} (1.9,6.9) $\times 10^{-7}$	29, 32, 34
R Cas	Mira	3100	176	10.5	8×10^{-7} 9×10^{-7} (0.5,2.2) $\times 10^{-6}$ 4×10^{-7}	3, 10, 18, 23
EP Aqr	SRb	3200	114	10.0	3.1×10^{-7} 1.2×10^{-7} (0.9,5.0) $\times 10^{-7}$	8, 18
NML Cyg	SRc	3800	620	33	8.7×10^{-5} 1.8×10^{-6} (0.6,2.3) $\times 10^{-4}$	18, 35
χ Cyg	Mira	2000	149	8.5	7×10^{-7} 4×10^{-7} (0.1,1.2) $\times 10^{-6}$ 2.4×10^{-7}	10, 17, 18, 20, 27

Notes. Column 1: target name; Col. 2: variability of the central star; Col. 3: effective temperature of the star; Col. 4: adopted distance to the object; Col. 5: expansion velocity of the circumstellar envelope; Col. 6: left: mass loss rate taken from the literature. Right: range of mass loss rates shown at left after being scaled to the values of d , v_{exp} and χ_{CO} used in this work. For those with only one previous estimation, the range cover a factor of 3 around that value after scaling. ^(a)Uncertain.

References. (1) Van de Sande et al. (2018) (2) Doan et al. (2017) (3) Maercker et al. (2016), (4) Santander-García et al. (2015), (5) Vickers et al. (2015), (6) Santander-García et al. (2015), (7) Danilovich et al. (2015), (8) Nhung et al. (2015), (9) He et al. (2014), (10) Ramstedt & Olofsson (2014), (11) Danilovich et al. (2014), (12) Khouri et al. (2014), (13) Justtanont et al. (2013), (14) Cox et al. (2012), (15) Choi et al. (2012), (16) Sánchez Contreras & Sahai (2012), (17) Schöier et al. (2011), (18) De Beck et al. (2010), (19) Decin et al. (2010), (20) Justtanont et al. (2010), (21) Ramstedt et al. (2009), (22) Meaburn et al. (2008), (23) Maercker et al. (2008), (24) Ramstedt et al. (2008), (25) Dinh-V-Trung et al. (2008), (26) Decin et al. (2007), (27) Teyssier et al. (2006), (28) Ramstedt et al. (2006), (29) Heras & Hony (2005), (30) Matsuura et al. (2005), (31) Woods et al. (2005), (32) Olofsson et al. (2002), (33) Alcolea et al. (2001), (34) Loup et al. (1993) and (35) Knapp et al. (1982).

Table D.2. continued.

Target name	Variability	T_{eff} (K)	d (pc)	v_{exp} (km s $^{-1}$)	$\dot{M}_{\text{Bibliography}}$ ($M_{\odot}$ yr $^{-1}$)		References
π Gru	SRb	2300	152	10.0	8.5×10^{-7} 7.7×10^{-7}	$(1.6, 4.9) \times 10^{-7}$	2, 7, 18
W Aql	Mira	2800	395	16.5	2.7×10^{-6} 1.3×10^{-5} 2.2×10^{-6} 2.5×10^{-6} 4×10^{-6}	$(0.2, 1.2) \times 10^{-5}$	10, 11, 18, 21, 28
WX Psc	Mira	2000	700	19.3	1.7×10^{-5} 4×10^{-5} 1.9×10^{-5} 6×10^{-6} 8.5×10^{-6}	$(0.4, 6.9) \times 10^{-5}$	10, 13, 18, 26, 35
V1300 Aql	Mira	2000	620	16.5	10^{-5} 4.5×10^{-6} 1.6×10^{-5}	$(0.4, 3.3) \times 10^{-5}$	7, 10, 18, 24
OH 231.8+4.2	Mira	2500	1500	15.0	1.6×10^{-4}	$(0.9, 2.8) \times 10^{-4}$	15, 33
OH 26.5+0.6	Mira	2750	1370	17.0	1.0×10^{-4} 9.7×10^{-6}	$(3, 0.8) \times 10^{-4}$	13, 18
IRAS 22036+5306	No	6900	4000	30.0	7.5×10^{-5} 7×10^{-6}	$(0.04, 1.3) \times 10^{-4}$	16
AFGL 6815	No	7000	2900	15.0	2.1×10^{-5} 3×10^{-5}	$(1.3, 4.7) \times 10^{-5}$	5, 9, 18, 31
IRAS 17347-3139	No	30000 ^a	3680 ^a	25.0	–	–	5, 30
NGC 6537	No	200000	1500	18.0	–	–	31
NGC 6302	No	250000	1170	10.0	1.5×10^{-4} 2.7×10^{-5}	$(0.09, 3.6) \times 10^{-4}$	4, 6, 22, 25

Table D.3. Results from our CO RD analysis (Sect. 6), including double-fit (hot and warm) components for NML Tau, χ Cyg, π Gru, W Aql, and IRAS 17347-3139.

Target name	d (pc)	v_{exp} (km s $^{-1}$)	r_{CO} (cm)	T_{rot} (K)	$N_{\text{CO}}^{\text{col}}$ (cm $^{-2}$)	M_{H_2} ($M_{\odot}$)	$\dot{M}$ ($M_{\odot}$ yr $^{-1}$)	Correction $_{M_{\text{H}_2}}$
RR Aql	530	9.0	1×10^{15}	460 ± 60	$(8.8 \pm 3.0) \times 10^{17}$	$(2.3 \pm 0.8) \times 10^{-5}$	7×10^{-7}	1.2
<i>o</i> Cet	110	8.1	6×10^{14}	530 ± 20	$(2.6 \pm 0.3) \times 10^{18}$	$(2.5 \pm 0.3) \times 10^{-5}$	10^{-6}	1.6
W Hya	98	7.5	4×10^{14}	550 ± 40	$(3.8 \pm 1.0) \times 10^{18}$	$(1.6 \pm 0.4) \times 10^{-5}$	9×10^{-7}	1.6
IRAS 20038-2722	197	5.4	4×10^{14}	500 ± 20	$(1.4 \pm 0.2) \times 10^{18}$	$(5.9 \pm 0.9) \times 10^{-6}$	3×10^{-7}	1.4
T Cep	190	5.5	1×10^{15}	370 ± 40	$(6.3 \pm 2.5) \times 10^{17}$	$(1.7 \pm 0.7) \times 10^{-5}$	3×10^{-7}	1.2
NML Tau	260	18.0	1×10^{15}	490 ± 20	$(5.9 \pm 1.0) \times 10^{18}$	$(1.6 \pm 0.3) \times 10^{-4}$	9×10^{-6}	1.5
NML Tau	260	18.0	1×10^{15}	370 ± 20	$(9.5 \pm 1.4) \times 10^{18}$	$(2.5 \pm 0.4) \times 10^{-4}$	1×10^{-5}	–
NML Tau	260	18.0	1×10^{15}	820 ± 210	$(1.0 \pm 0.9) \times 10^{18}$	$(2.7 \pm 2.4) \times 10^{-5}$	2×10^{-6}	–
R Dor	59	5.5	4×10^{14}	520 ± 20	$(1.8 \pm 0.2) \times 10^{18}$	$(7.7 \pm 0.8) \times 10^{-6}$	3×10^{-7}	1.5
TX Cam	380	18.5	2×10^{15}	240 ± 10	$(4.4 \pm 0.7) \times 10^{18}$	$(4.7 \pm 0.7) \times 10^{-4}$	10^{-5}	1.5
X Her	137	6.5	4×10^{14}	570 ± 50	$(8.0 \pm 1.8) \times 10^{17}$	$(3.4 \pm 0.8) \times 10^{-6}$	2×10^{-7}	1.2
IRAS 19474-0744	810	13.6	2×10^{15}	460 ± 40	$(2.1 \pm 0.5) \times 10^{18}$	$(2.3 \pm 0.5) \times 10^{-4}$	5×10^{-6}	1.3
T Mic	290	4.8	6×10^{14}	550 ± 30	$(1.8 \pm 0.3) \times 10^{18}$	$(1.7 \pm 0.3) \times 10^{-5}$	4×10^{-7}	1.6
R Cas	176	10.5	1×10^{15}	400 ± 20	$(1.2 \pm 0.1) \times 10^{18}$	$(3.1 \pm 0.4) \times 10^{-5}$	10^{-6}	1.2
EP Aqr	114	10.0	4×10^{14}	470 ± 20	$(1.3 \pm 0.2) \times 10^{18}$	$(5.6 \pm 0.6) \times 10^{-6}$	4×10^{-7}	1.2
NML Cyg	620	33.0	2×10^{15}	470 ± 20	$(1.2 \pm 0.2) \times 10^{19}$	$(1.3 \pm 0.2) \times 10^{-3}$	7×10^{-5}	1.6
χ Cyg	149	8.5	6×10^{14}	620 ± 10	$(3.7 \pm 0.3) \times 10^{18}$	$(1.2 \pm 0.1) \times 10^{-5}$	5×10^{-7}	1.6
χ Cyg	149	8.5	6×10^{14}	480 ± 20	$(4.9 \pm 0.4) \times 10^{18}$	$(1.6 \pm 0.2) \times 10^{-5}$	7×10^{-7}	–
χ Cyg	149	8.5	6×10^{14}	690 ± 30	$(2.3 \pm 0.2) \times 10^{18}$	$(7.3 \pm 1.5) \times 10^{-6}$	3×10^{-7}	–
π Gru	152	10.0	6×10^{14}	670 ± 20	$(4.0 \pm 0.6) \times 10^{18}$	$(1.3 \pm 0.2) \times 10^{-5}$	7×10^{-7}	1.4
π Gru	152	10.0	6×10^{14}	460 ± 20	$(7.1 \pm 1.1) \times 10^{18}$	$(2.3 \pm 0.2) \times 10^{-5}$	10^{-6}	–
π Gru	152	10.0	6×10^{14}	870 ± 30	$(1.3 \pm 0.2) \times 10^{18}$	$(4.2 \pm 0.7) \times 10^{-6}$	2×10^{-7}	–
W Aql	395	16.5	2×10^{15}	550 ± 10	$(2.9 \pm 0.2) \times 10^{18}$	$(1.0 \pm 0.1) \times 10^{-4}$	3×10^{-6}	1.2
W Aql	395	16.5	2×10^{15}	440 ± 10	$(3.9 \pm 0.3) \times 10^{18}$	$(1.4 \pm 0.1) \times 10^{-4}$	3×10^{-6}	–
W Aql	395	16.5	2×10^{15}	570 ± 20	$(2.3 \pm 0.6) \times 10^{18}$	$(7.9 \pm 2.0) \times 10^{-5}$	2×10^{-6}	–
WX Psc	700	19.3	2×10^{15}	560 ± 70	$(3.2 \pm 1.0) \times 10^{18}$	$(3.3 \pm 1.0) \times 10^{-4}$	10^{-5}	1.0
V1300 Aql	620	16.5	2×10^{15}	510 ± 20	$(1.8 \pm 0.2) \times 10^{18}$	$(1.9 \pm 0.2) \times 10^{-4}$	5×10^{-6}	1.0
OH 231.8+4.2	1500	15.0	4×10^{15}	240 ± 40	$(3.5 \pm 2.5) \times 10^{18}$	$(1.5 \pm 1.0) \times 10^{-3}$	2×10^{-5}	1.0
OH 26.5+0.6	1370	17.0	4×10^{15}	410 ± 100	$(2.4 \pm 1.8) \times 10^{18}$	$(1.0 \pm 0.8) \times 10^{-3}$	10^{-5}	1.0
IRAS 22036+5306	4000	30.0	6×10^{16}	280 ± 20	$(1.0 \pm 0.2) \times 10^{17}$	$(9.6 \pm 2.1) \times 10^{-3}$	2×10^{-5}	1.1
AFGL 6815	2900	15.0	6×10^{16}	310 ± 20	$(1.9 \pm 0.4) \times 10^{17}$	$(1.8 \pm 0.3) \times 10^{-2}$	10^{-5}	1.1
IRAS 17347-3139	3680	25.0	6×10^{16}	630 ± 20	$(5.3 \pm 0.7) \times 10^{17}$	$(5.0 \pm 0.6) \times 10^{-2}$	7×10^{-5}	1.0
IRAS 17347-3139	3680	25.0	6×10^{16}	480 ± 10	$(8.2 \pm 0.4) \times 10^{17}$	$(7.8 \pm 0.4) \times 10^{-2}$	10^{-4}	–
IRAS 17347-3139	3680	25.0	6×10^{16}	820 ± 40	$(1.7 \pm 0.4) \times 10^{17}$	$(1.6 \pm 0.4) \times 10^{-2}$	2×10^{-5}	–
NGC 6302	1170	10.0	6×10^{16}	280 ± 10	$(1.2 \pm 0.2) \times 10^{17}$	$(1.2 \pm 0.2) \times 10^{-2}$	6×10^{-6}	1.1
NGC 6537	1500	18.0	6×10^{16}	200 ± 10	$(1.5 \pm 0.4) \times 10^{17}$	$(1.4 \pm 0.4) \times 10^{-2}$	10^{-5}	1.0

Notes. Column 1: target name; Col. 2: distance to the source (d); Col. 3: expansion velocity of the gas (v_{exp}); Col. 4: characteristic radius of the CO-emitting region adopted (r_{CO}); Col. 5: rotational temperature (T_{rot}); Col. 6: column density of CO ($N_{\text{CO}}^{\text{col}}$); Col. 7: total mass of H $_2$ within the CO-emitting volume (M_{H_2}); Col. 8: mass-loss rate ($\dot{M} = M_{\text{H}_2} \times v_{\text{exp}}/r_{\text{CO}}$); and Col. 9: ratio between M_{H_2} after and before the opacity correction was applied.

Table D.4. Integrated fluxes of ^{12}CO lines for 26 sources studied in this work.

Line	λ_{ul} (μm)	A_{ul} (s^{-1})	E_u (K)	Flux ($10^{-16} \text{ W m}^{-2}$)	Flux ($10^{-16} \text{ W m}^{-2}$)	σ Cet	W Hya	Flux ($10^{-17} \text{ W m}^{-2}$)	IRAS 20038-2722	Flux ($10^{-17} \text{ W m}^{-2}$)	T Cep	Flux ($10^{-16} \text{ W m}^{-2}$)	NML Tau
14-13	186.0	2.74×10^{-4}	580.5	–	–	3.0 ± 0.1	2.2 ± 0.2	–	1.9 ± 0.4	–	–	–	3.4 ± 0.1
15-14	173.6	3.35×10^{-4}	663.4	–	–	3.3 ± 0.1	2.7 ± 0.2	–	2.9 ± 0.2	–	–	–	4.6 ± 0.1
16-15	162.8	4.05×10^{-4}	751.7	–	–	3.8 ± 0.1	9.0 ± 1.1^c	–	1.0 ± 0.4^a	–	–	–	3.4 ± 0.5
17-16	153.3	4.83×10^{-4}	845.6	–	–	3.6 ± 0.2	2.9 ± 0.3	–	2.8 ± 0.5	–	–	–	–
18-17	144.8	5.70×10^{-4}	945.0	–	–	4.2 ± 0.1	3.1 ± 0.2	–	3.8 ± 0.6^a	–	–	7.0 ± 0.5	4.4 ± 0.1
19-18	137.2	6.65×10^{-4}	1049.9	–	–	3.7 ± 0.3	3.3 ± 0.3^a	–	2.6 ± 0.6	–	–	5.6 ± 0.4	5.0 ± 0.1
20-19	130.4	7.70×10^{-4}	1160.2	–	–	4.2 ± 0.3	7.0 ± 0.4^a	–	3.2 ± 0.5	–	–	8.7 ± 1.0	4.1 ± 0.1
21-20	124.2	8.83×10^{-4}	1276.1	–	–	3.8 ± 0.6	2.5 ± 0.3	–	3.0 ± 0.6	–	–	6.0 ± 0.8	4.9 ± 0.2
22-21	118.6	1.01×10^{-3}	1397.4	–	–	19 ± 1.0^a	8.8 ± 0.5^a	–	13 ± 1.0^a	–	–	64 ± 1.0^a	3.7 ± 0.1
23-22	113.5	1.14×10^{-3}	1524.2	–	–	6.5 ± 0.5^a	16 ± 1.0^a	–	19 ± 1.0^a	–	–	32 ± 2.0^a	5.2 ± 0.3
24-23	108.8	1.28×10^{-3}	1656.5	–	–	3.2 ± 0.5	5.8 ± 1.1^a	–	12 ± 2.0^a	–	–	24 ± 0.1^a	–
25-24	104.5	1.43×10^{-3}	1794.3	–	–	1.7 ± 0.5^a	1.3 ± 1.0^a	–	2.7 ± 0.9	–	–	3.6 ± 0.2	3.6 ± 0.2
28-27	93.4	1.94×10^{-3}	2240.3	–	–	5.3 ± 0.4^a	6.9 ± 0.5^a	–	6.7 ± 0.8^a	–	–	2.4 ± 0.4	2.4 ± 0.4
29-28	90.2	2.13×10^{-3}	2399.9	–	–	2.4 ± 0.3^a	2.6 ± 0.5	–	2.5 ± 0.4	–	–	11 ± 0.1^a	11 ± 0.1^a
30-29	87.2	2.32×10^{-3}	2564.9	–	–	3.6 ± 0.8^a	1.3 ± 0.5	–	1.8 ± 0.8	–	–	2.5 ± 0.1^c	2.5 ± 0.1^c
31-30	84.4	2.52×10^{-3}	2735.3	–	–	4.7 ± 0.5^a	3.0 ± 0.6	–	3.8 ± 1.1^a	–	–	2.4 ± 0.2	2.4 ± 0.2
32-31	81.8	2.74×10^{-3}	2911.2	–	–	–	3.2 ± 0.7	–	–	–	–	5.5 ± 1.3^a	5.5 ± 1.3^a
33-32	79.4	2.95×10^{-3}	3092.5	–	–	–	–	–	–	–	–	1.7 ± 0.5	1.7 ± 0.5
34-33	77.1	3.18×10^{-3}	3279.2	–	–	–	–	–	–	–	–	2.2 ± 0.5	2.2 ± 0.5
35-34	74.9	3.40×10^{-3}	3471.3	–	–	–	–	–	–	–	–	–	–
36-35	72.9	3.64×10^{-3}	3668.9	–	–	–	–	–	–	–	–	–	–
37-36	70.9	3.88×10^{-3}	3871.8	–	–	–	–	–	–	–	–	–	–
38-37	70.9	4.12×10^{-3}	4080.1	–	–	–	–	–	–	–	–	–	–
39-38	67.3	4.37×10^{-3}	4293.7	–	–	–	–	–	–	–	–	–	–
40-39	65.7	4.61×10^{-3}	4512.8	–	–	–	–	–	–	–	–	–	–
41-40	64.1	4.86×10^{-3}	4737.2	–	–	–	–	–	–	–	–	–	–
42-41	62.6	5.11×10^{-3}	4966.9	–	–	–	–	–	–	–	–	–	–

Notes. Column 1: quantum numbers of the transition; Col. 2: wavelength corresponding to the emission lines; Cols. 3 and 4: integrated fluxes of the emission lines. ^(a)Blended line. ^(b)Bad determination of the continuum level. ^(c)Bad fit.

Table D.4. continued.

Line	λ_{ul} (μm)	Flux ($10^{-16} \text{ W m}^{-2}$)	Flux ($10^{-16} \text{ W m}^{-2}$)	Flux ($10^{-17} \text{ W m}^{-2}$)	Flux ($10^{-17} \text{ W m}^{-2}$)	Flux ($10^{-17} \text{ W m}^{-2}$)	Flux ($10^{-17} \text{ W m}^{-2}$)	Flux ($10^{-16} \text{ W m}^{-2}$)
		R Dor	TX Cam	X Her	IRAS 19474-0744	T Mic	R Cas	
14-13	186.0	2.6 ± 0.1	1.9 ± 0.1	4.5 ± 0.7	4.7 ± 0.7	1.9 ± 0.3	1.4 ± 0.1	
15-14	173.6	3.0 ± 0.2	2.0 ± 0.1	2.7 ± 0.4	5.5 ± 0.4	3.5 ± 0.2	1.6 ± 0.1	
16-15	162.8	69 ± 2.0^c	1.9 ± 0.1	2.9 ± 0.8	6.0 ± 0.4	3.3 ± 0.4	1.6 ± 0.1	
17-16	153.3	4.2 ± 0.4	2.1 ± 0.1	5.9 ± 0.8	6.8 ± 0.5	3.9 ± 0.3	1.7 ± 0.1	
18-17	144.8	5.1 ± 0.3	1.8 ± 0.1	8.5 ± 0.7^a	6.3 ± 0.5	4.6 ± 0.4	1.9 ± 0.1	
19-18	137.2	4.7 ± 0.5	1.6 ± 0.1	4.5 ± 0.8	5.4 ± 0.8	2.7 ± 2^c	1.5 ± 0.1	
20-19	130.4	4.7 ± 0.5	1.6 ± 0.2	4.4 ± 2.1	7.4 ± 0.5	5.3 ± 0.7	1.6 ± 0.1	
21-20	124.2	3.9 ± 0.4	9.0 ± 1.5	4.1 ± 0.6	6.0 ± 0.3	3.4 ± 0.3	1.4 ± 0.1	
22-21	118.6	13 ± 1.0^a	3.3 ± 0.2^a	10 ± 2^a	40 ± 1^a	21 ± 1^a	3.1 ± 0.1^a	
23-22	113.5	32 ± 1.0^a	7.9 ± 0.3^a	42 ± 1^a	42 ± 1^a	23 ± 1^a	13 ± 1^a	
24-23	108.8	6.4 ± 0.6	—	5.5 ± 1.8	8.3 ± 0.7	5.3 ± 0.9	1.1 ± 0.1	
25-24	104.5	—	—	—	11 ± 3^a	—	0.5 ± 0.1^a	
28-27	93.4	10 ± 1^a	—	4.5 ± 1.0	8.7 ± 1.5^a	—	2.1 ± 0.2^a	
29-28	90.2	3.6 ± 0.3	—	3.0 ± 1.4	—	5.0 ± 0.9	0.6 ± 0.1	
30-29	87.2	2.8 ± 0.8	—	5.4 ± 1.7	—	2.7 ± 1.0	1.0 ± 0.2	
31-30	84.4	6.3 ± 0.7^a	—	9.5 ± 2.4^a	—	5.5 ± 1.2^a	1.5 ± 0.2^a	
32-31	81.8	6.0 ± 1.6	—	—	—	—	0.9 ± 0.2^a	
33-32	79.4	—	—	—	—	—	—	
34-33	77.1	—	—	—	—	—	—	
35-34	74.9	—	—	—	—	—	—	
36-35	72.9	—	—	—	—	—	—	
37-36	70.9	—	—	—	—	—	—	
38-37	70.9	—	—	—	—	—	—	
39-38	67.3	—	—	—	—	—	—	
40-39	65.7	—	—	—	—	—	—	
41-40	64.1	—	—	—	—	—	—	
42-41	62.6	—	—	—	—	—	—	

Table D.4. continued.

Line	λ_{ul} (μm)	Flux ($10^{-17} \text{ W m}^{-2}$)	Flux ($10^{-16} \text{ W m}^{-2}$)	Flux ($10^{-16} \text{ W m}^{-2}$)	Flux ($10^{-16} \text{ W m}^{-2}$)	Flux ($10^{-16} \text{ W m}^{-2}$)	Flux ($10^{-16} \text{ W m}^{-2}$)	Flux ($10^{-16} \text{ W m}^{-2}$)
		EP Aqr	NML Cyg	χ Cyg	π Gru	W Aql	WX Psc	
14-13	186.0	6.4 ± 0.7	4.2 ± 0.2	2.4 ± 0.1	3.8 ± 0.1	3.5 ± 0.1	1.6 ± 0.1	
15-14	173.6	6.3 ± 0.5	4.5 ± 0.2	2.9 ± 0.1	3.6 ± 0.1	3.5 ± 0.1	1.2 ± 0.1	
16-15	162.8	23 ± 3^a	4.8 ± 0.5	3.2 ± 0.1	3.8 ± 0.1	4.3 ± 0.1	1.3 ± 0.2	
17-16	153.3	9.0 ± 0.8	5.4 ± 0.1	3.2 ± 0.1	4.5 ± 0.1	4.8 ± 0.1	1.8 ± 0.1	
18-17	144.8	12 ± 1^a	8.2 ± 0.1^a	3.9 ± 0.1	4.6 ± 0.1	4.7 ± 0.1	1.7 ± 0.1	
19-18	137.2	12 ± 1^a	4.6 ± 0.2	3.6 ± 0.1	4.6 ± 0.1	4.5 ± 0.1	1.1 ± 0.1	
20-19	130.4	8.5 ± 0.9	6.4 ± 0.3	4.4 ± 0.1	4.8 ± 0.1	5.6 ± 0.1	1.9 ± 0.2	
21-20	124.2	8.4 ± 1.0	3.9 ± 1.0	3.3 ± 0.1	4.7 ± 0.1	5.0 ± 0.0	1.1 ± 0.2	
22-21	118.6	3.2 ± 0.1^a	6.7 ± 0.7^c	4.1 ± 0.1	4.8 ± 0.1	4.9 ± 0.1	2.3 ± 0.1	
23-22	113.5	56 ± 1^a	35 ± 1^a	11 ± 1^a	9.1 ± 0.3^a	7.8 ± 0.2^a	9.2 ± 0.2^a	
24-23	108.8	8.2 ± 0.8	6.9 ± 0.2	4.1 ± 0.2	4.7 ± 0.1	4.0 ± 0.1	1.7 ± 0.2	
25-24	104.5	3.5 ± 2.7^a	7.9 ± 2.9^a	4.0 ± 0.2	4.8 ± 0.1	4.1 ± 0.2	–	
28-27	93.4	18 ± 1^a	26 ± 1^a	3.7 ± 0.1	3.9 ± 0.1	3.1 ± 0.1	5.4 ± 0.2^a	
29-28	90.2	11 ± 3^a	4.2 ± 0.3	3.9 ± 0.1	3.5 ± 0.1	3.3 ± 0.1	3.3 ± 0.9	
30-29	87.2	4.1 ± 1.2	2.4 ± 0.5	3.0 ± 0.1	3.9 ± 0.1	3.0 ± 0.2	0.81 ± 0.09	
31-30	84.4	16 ± 1^a	–	4.3 ± 0.1^a	4.4 ± 0.1^a	2.7 ± 0.2	–	
32-31	81.8	–	–	2.5 ± 0.1	2.9 ± 0.1	2.0 ± 0.1	–	
33-32	79.4	–	–	2.4 ± 0.2	3.0 ± 0.2	1.7 ± 0.2	–	
34-33	77.1	–	–	2.6 ± 0.2	2.6 ± 0.1	1.7 ± 0.1	–	
35-34	74.9	–	–	2.6 ± 0.4	6.7 ± 0.2^a	3.5 ± 0.3^a	–	
36-35	72.9	–	–	2.8 ± 0.3^a	2.4 ± 0.1	1.4 ± 0.3	–	
37-36	70.9	–	–	1.5 ± 0.2	1.7 ± 0.5	0.80 ± 0.18	–	
38-37	70.9	–	–	1.1 ± 0.2	1.9 ± 0.1	0.79 ± 0.15	–	
39-38	67.3	–	–	9.6 ± 0.7^a	3.5 ± 0.7^a	3.8 ± 0.3^a	–	
40-39	65.7	–	–	2.6 ± 0.6^a	1.8 ± 0.3	0.37 ± 0.11	–	
41-40	64.1	–	–	0.56 ± 0.17	1.4 ± 0.2	0.18 ± 0.17	–	
42-41	62.6	–	–	1.6 ± 0.5^a	0.94 ± 0.35	0.34 ± 0.12^a	–	

Table D.4. continued.

Line	λ_{ul} (μm)	Flux ($10^{-17} \text{ W m}^{-2}$)	Flux ($10^{-17} \text{ W m}^{-2}$)	Flux ($10^{-17} \text{ W m}^{-2}$)	Flux ($10^{-17} \text{ W m}^{-2}$)	Flux ($10^{-16} \text{ W m}^{-2}$)	Flux ($10^{-15} \text{ W m}^{-2}$)
		V1300 Aql	OH 231.8+4.2	OH 26.5+0.6	IRAS 22036+5306	AFGL 6815	IRAS 17347-3139
14-13	186.0	7.5 ± 0.4	4.1 ± 1.6	4.1 ± 1.3^a	11 ± 1^a	3.2 ± 0.1	0.90 ± 0.1
15-14	173.6	11 ± 1	28 ± 13	7.1 ± 1.0	6.4 ± 0.6	3.3 ± 0.1	1.1 ± 0.1
16-15	162.8	9.2 ± 1.6	23 ± 12	–	8.2 ± 1.0^a	2.5 ± 0.1	1.2 ± 0.1
17-16	153.3	12 ± 1	4.4 ± 1.8	11 ± 1	9.2 ± 0.9^a	2.3 ± 0.1	1.4 ± 0.1
18-17	144.8	14 ± 1	8.3 ± 1.7^a	15 ± 2	1.0 ± 0.2^a	2.5 ± 0.1	1.3 ± 0.1
19-18	137.2	8.2 ± 0.5	2.2 ± 1.2	0.70 ± 0.71^b	4.9 ± 1.7^a	2.0 ± 0.1	1.4 ± 0.1
20-19	130.4	9.5 ± 0.7	3.5 ± 1.5	7.1 ± 1.1	3.9 ± 0.5	2.2 ± 0.1	1.4 ± 0.1
21-20	124.2	6.9 ± 1.0^a	–	7.5 ± 1.7	5.4 ± 1.1^a	1.6 ± 0.1	1.4 ± 0.1
22-21	118.6	12 ± 1	–	4.8 ± 2.4	3.0 ± 0.8	1.2 ± 0.1	1.5 ± 0.1
23-22	113.5	44 ± 1^a	–	49 ± 5^a	6.6 ± 0.9^a	3.0 ± 0.1^a	2.2 ± 0.1^a
24-23	108.8	17 ± 1^a	–	15 ± 2	–	0.38 ± 0.07^c	1.3 ± 0.1
25-24	104.5	2.8 ± 3.0^a	–	–	–	0.91 ± 0.38^a	1.2 ± 0.1
28-27	93.4	–	–	–	–	0.43 ± 0.10	0.93 ± 0.02
29-28	90.2	6.0 ± 1.0	–	–	–	–	0.92 ± 0.02
30-29	87.2	5.6 ± 0.6	–	–	–	–	0.68 ± 0.02
31-30	84.4	4.6 ± 1.8^a	–	–	–	–	1.5 ± 0.1^a
32-31	81.8	3.5 ± 1.0	–	–	–	–	0.57 ± 0.02
33-32	79.4	4.4 ± 0.9^a	–	–	–	–	0.52 ± 0.03
34-33	77.1	2.7 ± 0.6	–	–	–	–	0.48 ± 0.02
35-34	74.9	–	–	–	–	–	0.47 ± 0.02
36-35	72.9	–	–	–	–	–	0.42 ± 0.03
37-36	70.9	–	–	–	–	–	0.54 ± 0.10^a
38-37	70.9	–	–	–	–	–	0.24 ± 0.04
39-38	67.3	–	–	–	–	–	0.34 ± 0.03
40-39	65.7	–	–	–	–	–	0.21 ± 0.03
41-40	64.1	–	–	–	–	–	0.26 ± 0.05
42-41	62.6	–	–	–	–	–	–

Table D.4. continued.

Line	λ_{ul} (μm)	Flux	Flux
		(10^{-16} W/m 2)	(10^{-16} W/m 2)
		NGC 6302	IRAS NGC 6537
14-13	186.0	9.9 ± 0.3	2.9 ± 0.3
15-14	173.6	9.0 ± 0.4	3.4 ± 0.2
16-15	162.8	8.4 ± 0.4	2.3 ± 0.2
17-16	153.3	8.3 ± 0.3	3.2 ± 0.2
18-17	144.8	9.7 ± 0.4	2.1 ± 0.1
19-18	137.2	5.5 ± 0.2	1.4 ± 0.1
20-19	130.4	6.5 ± 0.3	1.4 ± 0.1
21-20	124.2	4.2 ± 0.3	0.70 ± 0.06
22-21	118.6	3.2 ± 0.5	0.37 ± 0.07
23-22	113.5	2.8 ± 0.5	0.82 ± 0.31^a
24-23	108.8	1.7 ± 1.0^a	—
25-24	104.5	2.4 ± 0.3	—
28-27	93.4	—	—
29-28	90.2	—	—
30-29	87.2	—	—
31-30	84.4	—	—
32-31	81.8	—	—
33-32	79.4	—	—
34-33	77.1	—	—
35-34	74.9	—	—
36-35	72.9	—	—
37-36	70.9	—	—
38-37	70.9	—	—
39-38	67.3	—	—
40-39	65.7	—	—
41-40	64.1	—	—
42-41	62.6	—	—