Modeling the H$_2$O submillimeter emission in extragalactic sources*

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ABSTRACT

Recent observational studies have shown that H$_2$O emission at (rest) submillimeter wavelengths is ubiquitous in infrared galaxies, both in the local and in the early Universe, suggestive of far-infrared pumping of H$_2$O by dust in warm regions. In this work, models are presented that show that (i) the highest-lying H$_2$O lines ($E_{\text{upper}} > 400$ K) are formed in very warm ($T_{\text{dust}} \gtrsim 90$ K) regions and require high H$_2$O columns ($N_{\text{H}_2O} \gtrsim 3 \times 10^{15}$ cm$^{-2}$), while lower lying lines can be efficiently excited with $T_{\text{dust}} \sim 45$–75 K and $N_{\text{H}_2O} \sim (0.5–2) \times 10^{17}$ cm$^{-2}$; (ii) significant collisional excitation of the lowest lying ($E_{\text{upper}} < 200$ K) levels, which enhances the overall $L_{\text{H}_2O}/L_{\text{IR}}$ ratios, is identified in sources where the ground-state para-H$_2$O $1_{11}$–$0_{00}$ line is detected in emission; (iii) the H$_2$O-to-infrared (8–1000 μm) luminosity ratio is expected to decrease with increasing $T_{\text{dust}}$ for all lines with $E_{\text{upper}} \lesssim 300$ K, as has recently been reported in a sample of LIRGs, but increases with $T_{\text{dust}}$ for the highest lying H$_2$O lines ($E_{\text{upper}} > 400$ K); (iv) we find theoretical upper limits for $L_{\text{H}_2O}/L_{\text{IR}}$ in warm environments, owing to H$_2$O line saturation; (v) individual models are presented for two very different prototypical galaxies, the Seyfert 2 galaxy NGC 1068 and the nearest ultraluminous infrared galaxy Arp 220, showing that the excited submillimeter H$_2$O emission is dominated by far-infrared pumping in both cases; (vi) the $L_{\text{H}_2O}/L_{\text{IR}}$ correlation previously reported in observational studies indicates depletion or exhaustion time scales, $t_{\text{deq}} = \Sigma_{\text{gas}}/\Sigma_{\text{FR}}$, of $\lesssim 12$ Myr for star-forming sources where lines up to $E_{\text{upper}} = 300$ K are detected, in agreement with the values previously found for (U)LIRGs from HCN millimeter emission. We conclude that the submillimeter H$_2$O line emission other than the para-H$_2$O $1_{11}$–$0_{00}$ transition is pumped primarily by far-infrared radiation, though some collisional pumping may contribute to the low-lying para-H$_2$O $2_{02}$–$1_{11}$ line, and that collisional pumping of the para-$1_{11}$ and ortho-$2_{12}$ levels enhances the radiative pumping of the higher lying levels.

Key words. line: formation – galaxies: ISM – infrared: galaxies – submillimeter: galaxies

1. Introduction

With its high dipolar moment, extremely rich spectrum, and high level spacing (in comparison to those of other molecules with low-lying transitions at millimeter wavelengths), H$_2$O couples very well to the radiation field in warm regions that emit strongly in the far-IR. In extragalactic sources, excited lines of H$_2$O at far-IR wavelengths ($\lambda < 200$ μm) were detected in absorption with the Infrared Space Telescope (ISO; Fischer et al. 1999; González-Alfonso et al. 2004, 2008), and with Herschel/PACS (Pilbratt et al. 2010; Poglitsch et al. 2010) in Mrk 231 (Fischer et al. 2010), Arp 220 and NGC 4418 (González-Alfonso et al. 2012, G-A12). Modeling and analysis have demonstrated the ability of H$_2$O to be efficiently excited through absorption of far-IR dust-emitted photons, thus providing a powerful method for studying the strength of the far-IR field in compact/warm regions that are not spatially resolved at far-IR wavelengths with current (or foreseen) technology.

Herschel/SPIRE (Griffin et al. 2010) has enabled the observation of H$_2$O at submillimeter (hereafter submm, $\lambda > 200$ μm) wavelengths in local sources, where the excited (i.e., non-ground-state) lines are invariably seen in emission. In Mrk 231, lines with $E_{\text{upper}}$ up to 640 K were detected (van der Werf et al. 2010; González-Alfonso et al. 2010, hereafter G-A10), with strengths comparable to the CO lines. The H$_2$O lines have been also detected in other local sources (Rangwala et al. 2011; Pereira-Santaella et al. 2013), including the Seyfert 2 galaxy NGC 1068 (Spinoglio et al. 2012, S12). Furthermore, submm lines of H$_2$O have been detected in a dozen of high-$z$ sources (Impellizzeri et al. 2008; Omont et al. 2011; Lis et al. 2011; van der Werf et al. 2011; Bradford et al. 2011; Combes et al. 2012; Lupu et al. 2012; Bothwell et al. 2013), even in a $z = 6.34$ galaxy (Riechers et al. 2013). Recently, a striking correlation has been found between the submm H$_2$O luminosity ($L_{\text{H}_2O}$), taken from the $2_{02}$–$1_{11}$ and $2_{11}$–$2_{02}$ lines, and the IR luminosity ($L_{\text{IR}}$), including both local and high-$z$ ULIRGs (Omont et al. 2013, hereafter O13). Using SPIRE spectroscopy of local IR-bright galaxies and published data from high-$z$ sources, the linear correlations between $L_{\text{H}_2O}$ and $L_{\text{IR}}$ for five of the strongest lines, extending over more than three orders of magnitude in IR luminosity, has recently been confirmed (Yang et al. 2013, hereafter Y13). There are hints of an increase in $L_{\text{H}_2O}$ that is slightly faster than linear with $L_{\text{IR}}$ in some lines ($2_{11}$–$2_{02}$ and $2_{20}$–$2_{11}$) and in high-$z$ ULIRGs (O13). HCN is another key species that also shows a tight correlation with the IR luminosity, even though the excitation of the 1–0 transition is dominated by collisions with dense H$_2$ (Gao & Solomon 2004a,b).

The increasing wealth of observations of H$_2$O at submm wavelengths in both local and high-$z$ sources and the correlations discovered between $L_{\text{H}_2O}$ and $L_{\text{IR}}$ require a more extended analysis in parameter space than the one given in G-A10 for Mrk 231. In this work, models are presented to constrain the

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submillimeter wavelengths with blue arrows, and the far-IR H$_2$O pumping (absorption) lines with dashed-magenta arrows. The lines are numbered as listed in Table 1. The o-H$_2$O $3_2$–$2_1$ transition is not considered due to blending with CO (10–9) (G-A10), and the far-IR $2_{12}$–$1_{01}$ transition at 179.5 $\mu$m discussed in the text is also indicated in green for completeness.

physical and chemical conditions in the submm H$_2$O emitting regions in warm (U)LIRGs and to propose a general framework for interpreting the H$_2$O submm emission in extragalactic sources.

2. Excitation overview

At submm wavelengths, H$_2$O responds to far-IR excitation by emitting photons through a cascade process. This is illustrated in Fig. 1, where four far-IR pumping lines (at 101, 75, 58, and 45 $\mu$m) account for the radiative excitation of the submm lines (G-A10). The line parameters are listed in Table 1, where we use the numerals 1–8 to denote the submm lines. Lines 2–4, 5–6, 7, and 8 are pumped through the 101$^1$, 75, 58, and 45 $\mu$m far-IR transitions, respectively.

The ground-state line 1 has no analog pumping mechanism, so that the upper 111 level can only be excited through absorption of a photon in the same transition (at 269 $\mu$m) or through a collisional event. In the absence of significant collisional excitation, and if approximate spherical symmetry holds, line 1 will give negligible absorption or emission above the continuum (regardless of line opacity) if the continuum opacity at 269 $\mu$m is low or will be detected in absorption for significant 269 $\mu$m continuum opacities. This is supported by the SPIRE spectrum of Arp 220, in which line 1 is observed in absorption (Rangwala et al. 2011) and high submm continuum opacities are inferred (González-Alfonso et al. 2004; Downes & Eckart 2007; Sakamoto et al. 2008). Collisional excitation and thus high densities and gas temperatures are then expected in sources where line 1 is detected in emission (10 sources among 176, Y13), as in NGC 1068 (S12; see also Appendix A). Line 1 can then be collisionally excited in regions where the other lines do not emit owing to weak far-IR continuum; this effect has recently been observed in the intergalactic filament in the Stephan’s Quintet (Appleton et al. 2013).

If collisional excitation of the 111 and 212 levels dominates over absorption of dust photons at 269 and 179 $\mu$m (i.e., in very optically thin and/or high density sources), the submm H$_2$O lines 2–6 will be boosted because these 111 and 212 levels are the base levels from which the 101 and 75 $\mu$m radiative pumping cycles operate (Fig. 1). In addition, in regions of low continuum opacities but warm gas, collisional excitation of the para-H$_2$O level 202 from the ground 000 state can significantly enhance the emission of line 2. Therefore, the H$_2$O submm emission depends in general on both the far-IR radiation density in the emitting region and the possible collisional excitation of the low-lying levels (111, 212, and 202). Lines 7–8 require strong far-IR radiation density not only at 58–45 $\mu$m, but also at longer wavelengths, together with high H$_2$O column densities ($N_{\text{H}_2\text{O}}$) in order to significantly populate the lower backbone 313 and 414 levels.

3. Description of the models

The basic models for H$_2$O were described in G-A10 (see also references therein). Summarizing, we assume a simple spherically symmetric source with uniform physical properties ($T_{\text{dust}}$, $T_{\text{gas}}$, gas and dust densities, H$_2$O abundance), where gas and dust are assumed to be mixed. We only consider the far-IR radiation field generated within the modeled source, ignoring the effect of external fields (except for NGC 1068, Appendix A). The source is divided into a set of spherical shells where the statistical equilibrium level populations are calculated. The models are non-local, including line and continuum opacity effects. We assume an H$_2$O ortho-to-par ratio of 3. Line broadening is simulated by including a microturbulent velocity ($V_{\text{turb}}$), for which the FWHM velocity dispersion is $\Delta V = 1.67V_{\text{turb}}$. No systemic motions are included.
3.1. Mass absorption coefficient of dust

The black curve in Fig. 2 shows the dust mass opacity coefficient used in the current and our past models (González-Alfonso et al. 2008, 2010, 2012, 2013, 2014). Our values at 125 and 850 μm are $k_{125} = 30 \text{ cm}^2 \text{ g}^{-1}$ and $k_{850} = 0.7 \text{ cm}^2 \text{ g}^{-1}$, in good agreement with those derived by Dunne et al. (2003). Adopting a gas-to-dust ratio of $X = 100$ by mass, and using $\kappa_{100} = 44.5 \text{ cm}^2 \text{ g}^{-1}$, the column density of H nuclei is

$$N_H = \frac{X \tau_{100}}{m_H \kappa_{100}} = 1.3 \times 10^{24} \tau_{100} \text{ cm}^{-2},$$

where $\tau_{100}$ is the continuum optical depth at 100 μm.

For this adopted dust composition, the fit across the far-IR to submm (blue line in Fig. 2) indicates an emissivity index of $\beta = 1.85$, slightly steeper than the $\beta = 1.5-1.6$ values favored by Kövacs et al. (2010) and Casey (2012). The H$_2$O excitation is sensitive to the dust emission over a range of wavelengths (from 45 to 270 μm), but we find that our results on $L_{H_2O}/L_{IR}$ are insensitive to $\beta$ for $\beta$ values above 1.5 (Sect. 4.3.3).

3.2. Model parameters

As listed in Table 2, the model parameters we have chosen to characterize the physical conditions in the emitting regions are $T_{dust}$, the continuum optical depth at 100 μm along a radial path ($\tau_{100}$), the corresponding H$_2$O column density per unit of velocity interval ($N_{H_2O}/\Delta V$), the velocity dispersion $\Delta V$, $T_{gas}$, and the H$_2$ density ($n_{H_2}$). Fiducial values for some of these parameters are $\tau_{100} = 0.1$, $\Delta V = 100 \text{ km s}^{-1}$, $T_{gas} = 150 \text{ K}$, and $n_{H_2} = 3 \times 10^5 \text{ cm}^{-3}$. Collisional rates with H$_2$ were taken from Dubernet et al. (2009) and Daniel et al. (2011). Our relevant results are the line-flux ratios ($F_i/F_j$) and the luminosity ratios $L_{H_2O}/L_{IR}$.

Depending on the values of the above parameters, our models can be interpreted in terms of a single source or are better applied to each of an ensemble of clouds within a clumpy distribution. The radius of the modeled source is

$$R = \frac{N_{H_2}/n_{H_2}}{0.21} \times \frac{(\tau_{100})}{0.1} \times \left(\frac{10^5 \text{ cm}^{-3}}{n_{H_2}}\right) \text{ pc},$$

where Eq. (1) has been applied. The corresponding IR luminosity can be written as $L_{IR} = 4\pi R^2 \sigma T_{dust}^4 \gamma$, where $\gamma(T_{dust}, \tau_{100} \leq 1)$ accounts for the departure from a blackbody emission due to finite optical depths, ranging from $\gamma = 0.2$ for $T_{dust} = 50 \text{ K}$ and $\tau_{100} = 0.1$ to $\gamma = 0.9$ for $T_{dust} = 95 \text{ K}$ and $\tau_{100} = 1$. In physical units,

$$L_{IR} = 1.4 \times 10^5 \left(\frac{\tau_{100}}{0.1}\right)^2 \left(\frac{10^5 \text{ cm}^{-3}}{n_{H_2}}\right)^2 \left(\frac{T_{dust}}{55 \text{ K}}\right)^4 \times \left(\frac{\gamma}{0.2}\right),$$

in $L_{\odot}$, indicating that a model with $\tau_{100} \sim 0.1$ and moderate $T_{dust}$ should be considered as one of an ensemble of clumps to account for the typically observed IR luminosities of $\geq 10^{11} L_{\odot}$ (Y13). For very warm ($T_{dust} \sim 90 \text{ K}$) and optically thick ($\tau_{100} \sim 1$) sources with low average densities ($n_{H_2} = 3 \times 10^3 \text{ cm}^{-3}$), Eq. (3) gives $L_{IR} \sim 5 \times 10^{11} L_{\odot}$ and the model can be applied to a significant fraction of the circumnuclear region of galaxies where the clumps may have partially lost their individuality (Downes & Solomon 1998).

The velocity dispersion $\Delta V$ in our models can be related to the velocity gradient used in escape probability methods as $dV/dr \sim \Delta V/(2R)$, and using Eq. (2)

$$dV/dr \sim 238 \times \left(\frac{\Delta V}{100 \text{ km s}^{-1}}\right) \times \left(\frac{0.1}{\tau_{100}}\right) \times \left(\frac{n_{H_2}}{10^5 \text{ cm}^{-3}}\right) \text{ km s}^{-1} \text{ pc}^{-1},$$

defining $K_{vir}$ as the ratio of the velocity gradient relative to that expected in gravitational virial equilibrium, $K_{vir} = (dV/dr)/(dV/dr)_{vir}$, and using $(dV/dr)_{vir} \sim 10 \times (n_{H_2}/10^5 \text{ cm}^{-3})^{1/2} \text{ km s}^{-1} \text{ pc}^{-1}$ (Bryant & Scoville 1996; Goldsmith 2001; Papadopoulos et al. 2007; Hailey-Dunsheath et al. 2012), we obtain

$$K_{vir} \sim 23.8 \times \left(\frac{\Delta V}{100 \text{ km s}^{-1}}\right) \times \left(\frac{0.1}{\tau_{100}}\right) \times \left(\frac{n_{H_2}}{10^5 \text{ cm}^{-3}}\right)^{1/2}. \quad (5)$$

Values of $K_{vir}$ significantly above 1 and up to ~20, indicating non-virialized phases, have been inferred in luminous IR galaxies from both low- and high-J CO lines (e.g., Papadopoulos & Seaguest 1999; Papadopoulos et al. 2007; Hailey-Dunsheath et al. 2012). For clarity, the velocity dispersion is rewritten in terms of $K_{vir}$ as

$$\Delta V = 42 \times \left(\frac{K_{vir}}{10}\right) \times \left(\frac{\tau_{100}}{0.1}\right) \times \left(\frac{10^5 \text{ cm}^{-3}}{n_{H_2}}\right)^{1/2} \text{ km s}^{-1}, \quad (6)$$

which shows that, for compact and dense clumps ($\tau_{100} = 0.1$, $n_{H_2} = 3 \times 10^5 \text{ cm}^{-3}$), $\Delta V \sim 25 \times (K_{vir}/10) \text{ km s}^{-1}$ and the typical observed linewidths (~300 km s$^{-1}$) are caused by the galaxy rotation pattern and velocity dispersion of clumps. In contrast, for optically thick sources with low densities ($\tau_{100} = 1$, $n_{H_2} \leq 10^4 \text{ cm}^{-3}$), $\Delta V \geq 130 \text{ km s}^{-1}$ is required for $K_{vir} \geq 1$.

Instead of calculating $\Delta V$ for each model according to Eq. (6), which would involve a “universal” $K_{vir}$ independent of
the source characteristics\textsuperscript{4}, we have used $\Delta V = 100$ km s\textsuperscript{-1} for comparison purposes between models (in Sect. 4.3.5 we also consider models with constant $K_{vir}$). Nevertheless, results can be easily rescaled to any other value of $\Delta V$ as follows. For given $T_{dust}$ and $\tau_{100}$, the relative level populations, the line opacities, and thus the H$_2$O line-flux ratios ($F_i/F_j$) depend on $N_{H_2O}/\Delta V$, while the luminosity ratios $L_{H_2O}/L_{IR}$ are proportional to $\Delta V$. Therefore, for any $\Delta V$, identical results for $F_i/F_j$ are obtained with the substitution

$$N_{H_2O} \rightarrow N_{H_2O} \times \left(\frac{\Delta V}{100 \text{ km s}^{-1}}\right),$$

while $L_{H_2O}/L_{IR}$ should be scaled as

$$\frac{L_{H_2O}}{L_{IR}} \rightarrow \frac{L_{H_2O}}{L_{IR}} \times \left(\frac{\Delta V}{100 \text{ km s}^{-1}}\right).$$

Both the line-flux ratios ($F_i/F_j$) and the luminosity ratios $L_{H_2O}/L_{IR}$ are independent of the number of clumps ($N_c$) if the model parameters ($T_{dust}$, $\tau_{100}$, $T_{gas}$, $N_{H_2O}/\Delta V$, and $\Delta V$) remain the same for the cloud average. With the effective source radius defined as $R_{eff} = N_c^{1/2} R$, both the line and continuum luminosities scale as $\propto R_{eff}^2$. Therefore, if the effective source size is changed and all other parameters are kept constant, a linear correlation between each $L_{H_2O}$ and $L_{IR}$ is naturally generated, regardless of the excitation mechanism of H$_2$O. (For reference, however, all absolute luminosities below are given for $R_{eff} = 100$ pc.) The question, then, is what range of dust and gas parameters characterizes the sources for which the observed nearly linear correlations in lines 2–6 (O13, Y13) are observed. The detection rates of lines 1, 7, and 8 are relatively low, but the same trend is observed in the few sources where they are detected (Y13).

In the following sections, the general results of our models are presented, while specific fits to two extreme sources, Arp 220 and NGC 1068, are discussed in Appendix A.

4. Model results

4.1. General results

In Fig. 3, model results are shown in which $T_{dust}$ is varied from 35 to 115 K, $N_{H_2O}/\Delta V$ from 5 x $10^{14}$ to 5 x $10^{15}$ cm\textsuperscript{-2}/(km s\textsuperscript{-1}), $\tau_{100}$ from 0.1 to 1.0, and where collisional excitation with $n_{H_2} = 3 \times 10^3$ cm\textsuperscript{-3} and $T_{gas} = 150$ K is excluded (a–c) or included (d–f). Panels a1–f1 (top) show the expected SLED normalized to line 2, and panels a2–f2 (bottom) plot the corresponding $L_{H_2O}/L_{IR} \times (100$ km s\textsuperscript{-1}/$\Delta V$) ratios as a function of $T_{dust}$ and $L_{IR}$ (for $R_{eff} = 100$ pc; all points would move horizontally for different $R_{eff}$). The effect of collisional excitation is also illustrated in Fig. 4, where the H$_2$O submm fluxes of lines 2–6 relative to those obtained ignoring collisional excitation are plotted as a function of $n_{H_2}$ for $T_{gas} = 150$ K.

The first conclusion that we infer from Figs. 3a1–f1 is that the relative fluxes of lines 5–6 generally increase with increasing $T_{dust}$. These lines are pumped through the H$_2$O transition at $\lambda \sim 75$ mm (Fig. 1), thus requiring warmer dust than lines 2–4, which are pumped through absorption of 100 $\mu$m photons. The SLEDs obtained with $T_{dust} < 45$ K yield $F_5$ significantly above $F_6$, and are thus unlike those observed in most (U)LIRGS (Y13). The two peaks in the H$_2$O SLED (in lines 2 and 6) generally found in (U)LIRGS (Y13) indicate that the submm H$_2$O emission essentially samples regions with $T_{dust} \gtrsim 45$ K. Significant collisional excitation enhances line 4 relative to line 6 (Figs. 3d1–f1), thus aggravating the discrepancy between the $T_{dust} < 45$ K models and the observations.

Lines 7–8 provide stringent constraints on $T_{dust}$, $\tau_{100}$, and $N_{H_2O}/\Delta V$. Since line 6 is still easily excited even with moderately warm $T_{dust} \sim 55$ K, the 8/6 and 7/6 ratios are good indicators of whether very warm dust (>80 K) is exciting H$_2$O. Sources where lines 7–8 are detected (e.g., Mrk 231, Arp 220, and APM 08279) can be considered “very warm” on these grounds, with $N_{H_2O}/\Delta V \gtrsim 3 \times 10^{15}$ cm\textsuperscript{-2}/(km s\textsuperscript{-1}). Sources where lines 7–8 are not detected to a significant level, but where the SLED still shows a second peak in line 6, are considered “warm”, i.e. with $T_{dust}$ varying between ~45 and 80 K, and $N_{H_2O}/\Delta V \sim (5-20) \times 10^{14}$ cm\textsuperscript{-2}/(km s\textsuperscript{-1}).

Sources in which lines 2–6 are not detected to a significant level, that do not show a second peak in line 6, or for which the H$_2$O luminosities are well below the observed $L_{H_2O}/L_{IR}$ correlation are considered “cold”. These sources are characterized by very optically thin and extended continuum emission, and/or with low $N_{H_2O}$ (these properties likely go together). Such sources include starbursts like M82 (Y13), where the continuum is generated in PDRs and are physically very different from the properties of “very warm” sources like Mrk 231 (G-A10).

In the models that neglect collisional excitation (a1–c1), line 1 is predicted to be in absorption, transitioning to emission in warm/dense regions where it is collisionally excited (d1–f1), as previously argued. Its strength will also depend on the continuum opacity, which should be low enough to allow the line to emit above the continuum. Direct collisional excitation from the ground state in regions with warm gas but low $\tau_{100}$ efficiently populates level $2_{02}$, so that the 2/3, 2/4, 2/5, and 2/6 ratios strongly increase with increasing $n_{H_2}$ (Fig. 4a). As advanced in Sect. 2, collisional excitation also boosts all other submm lines for moderate $T_{dust}$ owing to efficient pumping of the base levels $2_{12}$ and $1_{11}$; radiative trapping of photons emitted in the ground-state transitions increases the chance of absorption of continuum photons in the 101 and 75 $\mu$m transitions. Nevertheless, collisional excitation is negligible for high $\tau_{100}$ and high $T_{dust}$ (Fig. 4b).

4.2. Predicted line ratios

In sources where lines 7 and 8 are not detected, the 6/4 flux ratio is the most direct indication of the hardness of the far-IR radiation field seen by the H$_2$O gas responsible for the observed emission. Since line 4 is pumped through absorption of 101 $\mu$m photons and line 6 by 75 $\mu$m photons (Fig. 1), one may expect a correlation between the 6/4 ratio and the 75- to 100 $\mu$m far-IR color, $f_{55}/f_{100}$. As shown in Fig. 5a, our models indeed show a steep increase in the 6/4 ratio with $T_{dust}$ for fixed $\tau_{100}$ and $N_{H_2O}$. The averaged observed 6/4 ratio of $\sim$1.45–1.7 in strong-AGN and HII+mild-AGN sources (Y13) indicates, assuming an optically thin continuum (Fig. 5a), $T_{dust} \approx 55–75$ K and $f_{55}/f_{100} \approx 1.5–1.8$. For the case of high $\tau_{100}$ and $N_{H_2O}/\Delta V$, the averaged 6/4 ratio is consistent with lower $T_{dust}$ and $f_{55}/f_{100} = 1–1.2$.

\textsuperscript{4} We may expect $K_{vir} > 1$ for clouds in a clumpy distribution due to the gravitational potential of the galaxy and external pressure (Papadopoulos & Seaga 1999), but $K_{vir} \sim 1$ may be more appropriate for sources where the clouds have coalesced and the resulting (modeled) structure can be considered more isolated. However, $K_{vir} > 1$ in case of prominent outflows.
In general, the 6/4 ratio indicates $T_{\text{dust}} \approx 45 - 80$ K. Similarly, the 6/2 ratio is also sensitive to $T_{\text{dust}}$, as shown in Fig. 5b. The observed averaged 6/2 ratio of $\approx 1$–1.2 is compatible with $T_{\text{dust}}$ somewhat lower than estimated from the 6/4 ratio. This is attributable to the effects of collisional excitation of the 202 level (thus enhancing line 2 over line 6, see Fig. 4a and magenta symbols in Fig. 5b), or to the contribution to line 2 by an extended, low $T_{\text{dust}}$ component.

5 Such high $T_{\text{dust}}$ can be explained in the optically thin case as follows: first, the para-111 level is more easily populated through radiation than the ortho-212 level, because the $B_{\text{h}}/A_{\text{h}}$ ratio for the 111–000 transition is a factor 6 higher than for the 212–101 transition (which is the Einstein coefficients for photo absorption and spontaneous emission). Second, the $B_{\text{h}}$ coefficient of the para-202–111 pumping transition is a factor of $\approx 2.3$ higher than that of the ortho-311–212 pumping transition. Taking into account an ortho-to-para ratio of 3, a 6/4 ratio of 1 is obtained for $J_{111}/J_{202}=4.5$ ($J_1$ is the mean specific intensity at wavelength $\lambda$), which requires $T_{\text{dust}} \approx 45$ K.

There is, however, no observed correlation between the 6/4 ratio and $f_{68}/f_{100}$ (Y13), which should still show a correlation (though maybe less pronounced) than the expected correlation with $f_{68}/f_{100}$. As we argue in Sect. 4.3, this lack of correlation suggests that the observed far-IR $f_{68}/f_{100}$ colors, and in particular the observed $f_{68}$ fluxes, are not dominated by the warm component responsible for the H2O emission. Indeed, current models for the continuum emission in (U)LIRGs indicate that the flux density at 100 $\mu$m is dominated by relatively cold dust components ($T_{\text{dust}} \sim 30$ K) (e.g., Dunne et al. 2003; Kovacs et al. 2010; Casey 2012). The observed H2O emission thus arises in warm regions whose continuum is hidden within the observed far-IR emission, but may dominate the observed SED at $\lambda \lesssim 50$ $\mu$m (e.g., Casey 2012, see also Sect. 4.3.1).
case of high N at F in Table 2 by Y13, though a) on the details (weights) of the average computation. τ low and substantial columns of H2O and dust. This indicates that fluxes relative to the model that ignores collisional excitation.

- In optically thin conditions, we expect a 6 > 1 ratio of F6/F5 = 1.16 (Fig. 6). This is a lower limit, because in case of high NH2O/ΔV and/or high Tdust and τ100, absorption of line 5 emitted photons that can eventually be reemitted through the 312 − 221 transition, or absorption of continuum photons in the H2O 423−312 transition, will decrease the strength of line 5 relative to line 6.

- Although with significant dispersion, overall data for HII-mild AGN sources indicate F6/F5 ≈ 1.2 (Y13), consistent with the optically thin limit; examples of this galaxy population are NGC 1068 and NGC 6240 (Spinoglio et al. 2012; Meijerink et al. 2013). There are, however, sources like Arp 220 and Mrk 231 with F6/F5 = 1.6, favoring warm dust (>55 K) and substantial columns of H2O and dust. This indicates that sources in both the optically thin and optically thick regimes are H2O emitters.

- In optically thin conditions and with moderate Tdust, lines 2−4, together with the pumping 220−111 101 µm transition, form a closed loop (Fig. 1) where statistical equilibrium of the level populations implies equal fluxes for the three submm lines (Figs. 3a1−c1). The rise in Tdust and τ100, however, increases the chance of line absorption in the strong 221−111 transition at 90 µm, thus decreasing the flux of line 3 relative to both line 2 and 4. Consequently, the F2/F3 ratio is expected to increase from ≈1 (for low τ100) to ≈2 (for τ100 ≈ 1 and NH2O/ΔV ≈ 1017 cm−2/(km s−1)), consistent with the relatively high values found in the warm Mrk 231 and APM 08279 (Y13). If collisional excitation is important (Figs. 3d−f), F2/F3 is also expected to increase because collisions mainly boost the lower lying line 2 (Fig. 4a).

- One interesting caveat is, however, the behavior of the 4/3 ratio, because increasing Tdust and/or NH2O is predicted to increase F2/F3 but maintains F6/F3 > 1 (Figs. 3a1−c1). In Mrk 231, the high F2/F3 ratio and mostly the detection of lines 7−8 indicate very warm dust (G−A10), but the relatively low F6/F3 ≤ 1 observed in the source does not match this simple scheme. The problem is exacerbated with the 6/2 ratio, which is also expected to increase with increasing Tdust and τ100 to ≈1.5 (Fig. 5), but Mrk 231 shows F6/F2 ≈ 1. Nevertheless, the problem can be solved if source structure is invoked. A composite model where a very warm component accounts for the high-lying lines and a
colder (dust) component enhances lines 2–4 (with probable contribution from collisionally excited gas, as suggested by the high velocity interval is $N_{\text{H}_2\text{O}}/\Delta V = 10^{13}$ cm$^{-2}$/(km s$^{-1}$) (green, blue, and magenta curves) and $N_{\text{H}_2\text{O}}/\Delta V = 5 \times 10^{15}$ cm$^{-2}$/(km s$^{-1}$) (red and black curves).

**4.3. The $L_{\text{H}_2\text{O}} - \lambda_{\text{IR}}$ correlations**

4.3.1. $\text{H}_2\text{O}$ and the observed SED

It has long been recognized that single-temperature graybody fits to galaxy SEDs at far-IR wavelengths often underpredict the observed emission at $\lambda < 50$ \(\mu\)m. Therefore, multicomponent fitting, based on, for example, a two-temperature approach, a power-law mass-temperature distribution, a power-law mass-intensity distribution, or a single cold dust temperature graybody with a mid-IR power law (Dunne et al. 2003; Kóvacs et al. 2010; Dale & Helou 2002; Casey 2012), is required to match the full SED from the mid-IR to millimeter wavelengths. Our single-temperature model results on the $\text{H}_2\text{O}$ SLED favors $T_{\text{dust}} \geq 45$ K (Sect. 4.2), significantly warmer than the cold dust temperatures (<40 K) that account for most of the observed far-IR emission in luminous IR galaxies, indicating that the $\text{H}_2\text{O}$ submm emission primarily probes the warm region(s) of galaxies where the mid-IR (20–50 \(\mu\)m) emission is generated (see footnote 5).

Relative to the total IR emission of a galaxy, $L_{\text{IR}}$, the contribution to the luminosity by a given $T_{\text{dust}}$ component is $f_i = L_{\text{H}_2\text{O}}/L_{\text{IR}}$, and the observed $\text{H}_2\text{O}$-to-IR luminosity ratio is

$$\frac{L_{\text{H}_2\text{O}}}{L_{\text{IR}}} = \sum_i f_i \left( \frac{L_{\text{H}_2\text{O}}}{L_{\text{IR}}} \right)_i = f_{\text{warm}} \left( \frac{L_{\text{H}_2\text{O}}}{L_{\text{IR}}} \right)_{\text{warm}} + f_{\text{cold}} \left( \frac{L_{\text{H}_2\text{O}}}{L_{\text{IR}}} \right)_{\text{cold}}$$

(9)

where $(L_{\text{H}_2\text{O}}/L_{\text{IR}})_i$ are the values plotted in Figs. 3a2–f2 (for $\Delta V = 100$ km s$^{-1}$), and the problem is grossly simplified by considering only two “warm” and “cold” components. From the comparison of the observed average SLED (Y13) with our models, we infer that the contribution by the cold component to $L_{\text{H}_2\text{O}}/L_{\text{IR}}$ is small, even though $j_{\text{cold}}$ may be high. Since our modeled $L_{\text{IR}}$ emission from the warm component is thus only a fraction, $f_{\text{warm}}$, of the total IR budget, the modeled $L_{\text{H}_2\text{O}}/L_{\text{IR}}$ ratios in Figs. 3a2–f2 should be considered upper limits. The value of $f_{\text{warm}}$ can only be estimated by fitting the individual SEDs.

4.3.2. $\text{H}_2\text{O}$ emission and monochromatic luminosities

The $\text{H}_2\text{O}$ submm emission of lines 2–6 essentially involves two excitation processes, that of the base level (212 for ortho and 111 for para-$\text{H}_2\text{O}$) and absorption in the transitions at 75 \(\mu\)m (ortho) or 101 \(\mu\)m (para, Fig. 1). If collisional excitation is unimportant, the excitation of the base levels is also produced by absorption of dust-emitted photons in the corresponding transitions, i.e., in the $2_{12} - 1_{01}$ line at 179 \(\mu\)m (ortho) or $1_{11} - 0_{01}$ at 269 \(\mu\)m (para). In optically thin conditions and for fixed $N_{\text{H}_2\text{O}}$ and $\Delta V$, our models then show a linear correlation between the $\text{H}_2\text{O}$ luminosities $L_{\text{H}_2\text{O}}$ and the product of the continuum monochromatic luminosities responsible for the excitation, $L_{179} \times L_{269}$ (ortho) or $L_{269} \times L_{101}$ (para). This linear correlation is illustrated in Fig. 7 for line 6. The linear correlation, however, breaks down when the line becomes optically thick or when collisional excitation becomes important (in which case, $L_{\text{H}_2\text{O}}$ is independent of $L_{179(269)}$).
cold dust. However, the continuum at $\lambda = 60 \mu m$ may still be contaminated to some extent, in which case the data points in Fig. 8 will move toward the left. We also recall that the $L_{H_2O}/L_{IR}$ values are upper limits.

The first conclusion inferred from Fig. 8 is that the range of $f_{25}/f_{60}$ colors measured by Y13 (between the dashed lines) matches $T_{dust}$ in the ranges favored by the observed $H_2O$ line flux ratios, that is, 50–75 K and optically thin conditions ($T_{100} \sim 0.1$) and also $T_{dust} = 60–95$ K and $T_{100} = 1.0$. This indicates that the warm environments responsible for the $H_2O$ emission are best traced in the continuum in this wavelength range, but also that the $f_{25}/f_{60}$ color alone involves degeneracy in the dominant $T_{dust}$ and $T_{100}$ responsible for the mid-IR continuum emission. As shown in Sect. 4.2, the first set of conditions can explain the line ratios 2–6 in warm sources (where lines 7–8 are not detected to a significant level), while the second set is required to explain the $H_2O$ emission in very warm sources (with detection of lines 7–8).

Second, it is also relevant that the $L_{H_2O}/L_{IR}$ values differ by a factor $\lesssim 2$ between models with warm dust in the optically thin regime ($T_{dust} = 55$ K, $T_{100} = 0.1$, $N_{H_2O}/AV = 10^{15}$ cm$^{-2}$(km s$^{-1}$)) and those with very warm dust in the optically thick regime with high $H_2O$ columns ($T_{dust} = 95$ K, $T_{100} = 1$, $N_{H_2O}/AV = 5 \times 10^{15}$ cm$^{-2}$(km s$^{-1}$)), potentially explaining why sources with different physical conditions show similar $L_{H_2O}/L_{IR}$ ratios (Y13).

Third, in optically thin conditions ($T_{100} \sim 0.1$) and if collisional excitation is unimportant, the models with constant $N_{H_2O}/AV = 10^{15}$ cm$^{-2}$(km s$^{-1}$) (blue symbols) predict a slow decrease in $L_{2-4}/L_{IR}$ and a nearly constant $L_{6-0}/L_{IR}$ with increasing $f_{25}/f_{60}$, as argued above. This behavior, however, fails to match the observed trends (Y13), as $L_{2-4}/L_{IR}$ and $L_{6-0}/L_{IR}$ decrease by factors of $\sim 2$ and $\sim 3$, respectively, when $f_{25}/f_{60}$ increases from $\lesssim 0.08$ to $\lesssim 0.15$. When collisional excitation is included (magenta symbols), the $L_{2-4}/L_{IR}$ ratios show a stronger dependence on $f_{25}/f_{60}$, but $L_{6-0}/L_{IR}$ still changes only slightly with $f_{25}/f_{60}$.

Similarly, optically thin models with varying $T_{dust}$ but constant $T_{100}$, $N_{H_2O}/AV$, and $AV$ cannot account for the observed $L_{H_2O}/L_{IR}$–$f_{25}/f_{60}$ trend. This indicates that, in optically thin galaxies, parameters other than $T_{dust}$ are systematically varied when $f_{25}/f_{60}$ is increased and that optically thick sources also contribute to the observed trend:

(i) Galaxies in the optically thin regime (with $T_{100} < 1$) are predicted to show a very steep dependence of $L_{H_2O}/L_{IR}$ on $T_{100}$ for constant $T_{dust}$ and $N_{H_2O}/(\Delta V T_{100}$) (that is, for constant $H_2O$ abundance), with higher $T_{100}$ implying lower $f_{25}/f_{60}$. We illustrate this point in Fig. 8 with the red squares, corresponding to $T_{dust} = 55$ and 65 K and $N_{H_2O}/(\Delta V T_{100}) = 5 \times 10^{15}$ cm$^{-2}$(km s$^{-1}$), with $T_{100}$ ranging from 0.1 to 0.3. Therefore, we expect that the observed increase in $f_{25}/f_{60}$ is not only due to an increase in $T_{dust}$ from source to source, but also to variations in $T_{100}$ in the optically thin regime. Examples of galaxies in this regime are the AGNs NGC 6240 and NGC 1068 (see also Appendix A).

(ii) In the optically thick regime ($T_{100} \gtrsim 1$), galaxies are also predicted to show a relatively steep variation in $L_{H_2O}/L_{IR}$ with $f_{25}/f_{60}$ due to increasing $T_{dust}$ (black symbols in Fig. 8) because the $H_2O$ lines saturate and their luminosities flatten with increasing monochromatic luminosities (Fig. 7). Extreme examples of this galaxy population are Arp 220 and Mrk 231. Line saturation also implies that the $L_{H_2O}/L_{IR}$ ratios are not much higher than in the optically thin case.

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4.3.3. The $L_{H_2O}/L_{IR}$ Ratios and $T_{dust}$

The above considerations are relevant for our understanding of the behavior of the modeled $L_{H_2O}/L_{IR}$ values with variations in $T_{dust}$. In the optically thin case and with collisional excitation ignored, the double dependence of $L_{H_2O}$ on two monochromatic luminosities implies that $L_{H_2O}$ is (nearly) proportional to $L_{IR}$. Our predicted SEDs indicate that, for small variations $T_{dust}$ around 55 K, $L_{250} \propto L_{IR}^{0.7}$ and $L_{100} \propto L_{IR}^{1.3}$, respectively, for the para-$H_2O$ lines 2–4, $L_{2-4} \propto L_{IR}^{0.8}$ in optically thin conditions, slightly slower than linear. For the ortho lines, $L_{1-0} \propto L_{IR}^{1.3}$ and $L_{75} \propto L_{IR}^{2.1}$, so that $L_{5-6} \propto L_{IR}$. This explains why, in Figs. 3a–b, the $L_{2-4}/L_{IR}$ ratios show a slight decrease with increasing $T_{dust}$ above 55 K, while $L_{5-6}/L_{IR}$ versus $T_{dust}$ attain a maximum at $T_{dust} \approx 55$ K in optically thin models that omit collisional excitation. These results are robust against variations in the spectral index of dust down to $\beta = 1.5$ (Sect. 3.1).

In Fig. 8 we show the $L_{H_2O}/L_{IR}$ ratios (with $\Delta V = 100$ km s$^{-1}$; $L_{H_2O}/L_{IR} \propto \Delta V$) for lines 2, 4, and 6 as a function of the $f_{25}/f_{60}$ color. The observed $f_{25}/f_{60}$ was used by Y13 to characterize the $H_2O$ emission and is especially relevant given that the $H_2O$ submm emission arises in warm regions in which the mid-IR continuum emission is not severely contaminated by
even if much higher \( N_{\text{H}_2\text{O}}/\Delta V = 5 \times 10^{15} \text{ cm}^{-2}/(\text{km s}^{-1}) \) are present, and the corresponding ratios are consistent with the observed values to within the uncertainties in \( f_{\text{warm}} \). The presence of even warmer dust (>100 K) with significant contribution to \( L_{\text{IR}} \) will further decrease \( L_{\text{H}_2\text{O}}/L_{\text{IR}} \) (Y13).

In summary, the steep decrease in \( L_{\text{H}_2\text{O}}/L_{\text{IR}} \) at \( f_{\text{SS}}/f_{\text{ISO}} \approx 0.1-0.15 \) measured by Y13 is consistent with both types of galaxies (with optically thin and optically thick continuum) populating the diagram and suggests that the observed variations in \( f_{\text{SS}}/f_{\text{ISO}} \) are not only due to variations in \( T_{\text{dust}} \) but also to variations in \( T_{\text{eff}} \) in the optically thick regime. At the other extreme, the optically thick (saturated) and very warm galaxies are also expected to show a decrease in \( L_{\text{H}_2\text{O}}/L_{\text{IR}} \) with increasing \( T_{\text{dust}} \) (and \( f_{\text{SS}}/f_{\text{ISO}} \), as anticipated by Y13. To distinguish between both regimes for a given galaxy, the line ratios (specifically \( F_6/F_5 \), Sect. 4.2) and mostly the detection of lines 7–8 or the detection of high-lying \( \text{H}_2\text{O} \) absorption lines at far-IR wavelengths are required. The observations reported by Y13 indicate that these optically thick and warm components (diagnosed by the detection of lines 7–8) are present in at least ten sources. At least in NGC 1068 the upper limits on lines 7–8 are stringent (S12), allowing us to infer optically thin conditions.

### 4.3.4. Line saturation and a theoretical upper limit to \( L_{\text{H}_2\text{O}}/L_{\text{IR}} \)

Saturation of the \( \text{H}_2\text{O} \) submm lines in optically thick (\( \tau_{100} \approx 1 \)) sources implies that there is an upper limit on \( L_{\text{H}_2\text{O}}/L_{\text{IR}} \times (100 \text{ km s}^{-1}/\Delta V) \) that, in the absence of significant collisional excitation, cannot be exceeded. In Fig. 9, the \( L_{\text{H}_2\text{O}}/L_{\text{IR}} \times (100 \text{ km s}^{-1}/\Delta V) \) ratios for lines 2, 4, and 6 are plotted as a function of \( \tau_{100} \) for the most favored \( T_{\text{dust}} \) range of 55–95 K and \( N_{\text{H}_2\text{O}}/\Delta V = (1-5) \times 10^{15} \text{ cm}^{-2}/(\text{km s}^{-1}) \). In optically thin conditions (\( \tau_{100} \leq 0.1 \) for \( N_{\text{H}_2\text{O}}/\Delta V = 10^{15} \text{ cm}^{-2}/(\text{km s}^{-1}) \)) and without collisions, \( L_{\text{H}_2\text{O}}/L_{\text{IR}} \) scales linearly (for fixed \( \Delta V \)) with \( \tau_{100} \) because \( L_{\text{H}_2\text{O}}/L_{\text{IR}} \propto \tau_{100} \). For \( \text{H}_2\text{O} \) lines saturating and show a maximum at \( \tau_{100} \approx 0.5-1 \). Values of \( \tau_{100} \) significantly higher than unity are predicted to decrease \( L_{\text{H}_2\text{O}}/L_{\text{IR}} \). In very optically thick components of very warm sources, the submm lines are predicted to be observed in weak emission or even in absorption, especially in line 4. Arp 220 is a case in point (Sakamoto et al. 2008), in which the \( \text{H}_2\text{O} \) submm emission is expected to arise from a region that surrounds the optically thick nuclei (see Appendix A). For \( \Delta V = 100 \text{ km s}^{-1} \), the maximum attainable values of \( L_{\text{H}_2\text{O}}/L_{\text{IR}} \) (red curves) are \( 3.5 \times 10^{-5}, 4 \times 10^{-5}, \) and \( 7 \times 10^{-5} \) for lines 2, 4, and 6, respectively, comfortably higher than the values observed in any source by Y13. Recently, a value of \( L_2/L_{\text{IR}} = (4.3 \pm 1.6) \times 10^{-5} \) has been measured in the submillimeter galaxy SPT 0538-50, a gravitationally lensed dusty star-forming galaxy at \( z \approx 2.8 \) (Bothwell et al. 2013). Although the authors do not exclude differential lensing effects, which could affect the line-to-luminosity ratios, this value is still consistent with our upper limit, suggesting strong saturation in this source. In HFLS3 at \( z = 6.34 \), Riechers et al. (2013) have measured \( F_6/F_2 = 2.2 \pm 0.5 \) and \( F_6/F_5 = 2.6 \pm 0.8 \); within the uncertainties, these values are consistent with warm or very warm \( T_{\text{dust}} \geq 65 \text{ K} \) and high \( N_{\text{H}_2\text{O}} \) (Figs. 5, 6). The \( \text{H}_2\text{O} \) lines are most likely saturated in HFLS3 as is also indicated by the \( L_2/L_{\text{IR}} = (7.7 \pm 1.3) \times 10^{-5} \) ratio, which is still consistent with the strong saturation limit for warm \( T_{\text{dust}} \) given the very broad linewidth of the \( \text{H}_2\text{O} \) line (∼940 km s⁻¹; see Sect 3.2). O13 reported \( L_2/L_{\text{IR}} = (0.5-2) \times 10^{-5} \) in high-z ultra-luminous infrared galaxies, also consistent with the upper limit in Fig. 9 even for \( T_{\text{dust}} \approx 75 \text{ K} \) when taking the broad line widths of the \( \text{H}_2\text{O} \) lines into account. Line saturation and a relatively small contribution from cold dust to the infrared emission in these extreme galaxies are implied. With collisional excitation in optically thick environments with moderate \( T_{\text{dust}} \) but high \( N_{\text{H}_2\text{O}} \), the above \( L_{\text{H}_2\text{O}}/L_{\text{IR}} \) ratios (red dashed lines in Fig. 9) may even attain higher values, though the adopted \( \Delta V = 100 \text{ km s}^{-1} \) is too high for \( \tau_{100} < 0.3 \) and \( n_{\text{H}_2} = 3 \times 10^5 \text{ cm}^{-3} \) (Sect 3.2, Eq. (6)).

### 4.3.5. The correlation

The broad range in observed \( L_{\text{IR}} \) in luminous IR galaxies with \( \text{H}_2\text{O} \) emission may be attributable to varying the effective size of the emitting region. As noted in Sect. 3.2, varying \( R_{\text{vir}} \) (equivalent to varying the number of individual regions that contribute to \( L_{\text{IR}} \) or to increasing \( L_{\text{IR}} \) for a single source) is expected to generate linear \( L_{\text{H}_2\text{O}} - L_{\text{IR}} \) correlations if the other parameters (\( T_{\text{dust}}, \tau_{100}, T_{\text{gas}}, n_{\text{H}_2}, N_{\text{H}_2\text{O}}/\Delta V, \) and \( \Delta V \)) remain constant.

In Fig. 10 we show the \( L_2/L_{\text{IR}} \) ratio as a function of \( \tau_{100} \) for models with \( T_{\text{dust}} = 55 \text{ K} \) and \( T_{\text{dust}} = 75 \text{ K} \) that assume a constant \( \text{H}_2\text{O}-\text{to}-\text{dust} \) opacity ratio, that is, \( N_{\text{H}_2}\tau_{100} = 10^{18} \text{ cm}^2 \). According to Eq. (1), this corresponds to a constant \( \text{H}_2\text{O} \) abundance of \( 7.7 \times 10^{-7} \). Both models with \( \Delta V = 100 \text{ km s}^{-1} \) (independent of \( \tau_{100} \)), and \( \Delta V/\tau_{100} = 100 \text{ km s}^{-1} \) (corresponding to a constant \( K_{\text{vir}} = 1.3 \)) are shown. The figure illustrates that a supralinear correlation between \( L_{\text{H}_2\text{O}} \) and \( L_{\text{IR}} \) can be expected if, on average, \( \tau_{100} \) is an increasing function of \( L_{\text{IR}} \). If most sources with \( L_{\text{IR}} \approx 5 \times 10^{10} L_\odot \) were optically thin (\( \tau_{100} \approx 0.1 \)), and the high-z sources with \( L_{\text{IR}} \sim 10^{13} L_\odot \) (O13) were mostly
optically thick ($\tau_{100} \sim 1$), one would then expect $L_2 \propto L_{IR}^{1.3}$ from Fig. 10, which can account for the observed suprilinear correlation found by O13 and Y13. However, similar suprilinear correlations would then be expected for the other submm lines 3–6.

5. Summary of the model results for optically classified starbursts and AGNs

Following the classification of sources by Y13 into optically classified star-formation-dominated galaxies with possible mild AGN contribution (HII+mild AGN sources) and optically identified strong-AGN sources, we now consider these two groups separately.

5.1. HII+mild AGN sources

We focus here on those HII+mild AGN sources where lines 2–6 are detected but lines 7–8 are undetected (that is, “warm” sources as defined in Sect. 4.1). The average H$_2$O flux ratios reported by Y13 (their Table 2) indicate that (i) $F_6/F_2 \sim 1.2$, favoring $T_{dust} = 55$ K if there is no significant collisional excitation and $T_{dust} = 75$ K if the H$_2$O emission arises in warm and dense gas (Fig. 5); (ii) $F_6/F_5 \sim 1.2$, consistent with the optically thin regime (Fig. 6). For these $T_{dust}$, Fig. 11a shows the values of $N_{H_2O}$ for $\Delta V = 100$ km s$^{-1}$ required to explain the observed $L_{H_2O}/L_{IR}$ ratios, as a function of $\tau_{100}$. Models with included or excluded collisional excitation are considered. We recall that $\Delta V$ is the velocity dispersion of the dominant structure(s) that accounts for the H$_2$O emission (Sect. 3.2), and for the case of low $\tau_{100}$ and relatively high densities, Eq. (6) suggests $\Delta V < 100$ km s$^{-1}$ with the consequent increase in $N_{H_2O}$ (Fig. 10).

The decrease in $\tau_{100}$ implies the increase in $N_{H_2O}$ in optically thin conditions and when collisional excitation is unimportant. Our best fit models for the average SLED (big solid symbols) favor optically thin far-IR emission ($\tau_{100} \lesssim 0.3$). In Figs. 11b–e, the detailed comparison between the $\tau_{100} = 0.1$ models and the observations (Y13) is shown. Significant collisional excitation is not favored for $T_{dust} = 55$ K, since it would increase $F_2$ relative to $F_6$. In addition, these optically thin models have the drawback of overestimating $F_4/F_2$. Conversely, the $T_{dust} = 75$ K models favor significant collisional excitation in order to increase $F_2$ relative to $F_6$. The very optically thin models ($\tau_{100} \lesssim 0.05$) are also not favored given the very high amounts of H$_2$O required to explain (with no collisional excitation) the $L_{H_2O}/L_{IR}$ ratios.

In summary, $T_{dust} = 55–75$ K, $\tau_{100} \sim 0.1$, and $N_{H_2O} \sim (0.5–2) \times 10^{17}$ cm$^{-2}$ can explain the bulk of the H$_2$O submm emission in warm star-forming galaxies (Table 2). As shown in Fig. 8, $T_{dust} = 55$ K and $\tau_{100} = 0.1–0.2$ predict 25–to-60 μm flux density ratios of $f_{25}/f_{60} = (8.5–6.0) \times 10^{-2}$, in agreement with the observed values for the bulk of sources (Y13), while $T_{dust} = 75$ K and $\tau_{100} = 0.1–0.2$ predict $f_{25}/f_{60} = 0.42–0.30$ (close to the observed upper values). Assuming a gas-to-dust ratio of 100 by mass, $\tau_{100} \sim 0.1$ corresponds to a column density $N_{H_2O} = 3 \times 10^{20}$ cm$^{-2}$ and a hydrogen column density $N_H = 3 \times 10^{21}$ cm$^{-2}$, corresponding to a column density $N_H$ of $10^{22}$ cm$^{-2}$, which is consistent with the observed H$_2$O column densities.

Fig. 10. Modeled $L_2/L_{IR}$ ratio as a function of $\tau_{100}$. Squares and triangles indicate $T_{dust} = 55$ and 75 K, respectively. In all models, collisional excitation is included with $T_{gas} = 150$ K and $n_H = 3 \times 10^5$ cm$^{-3}$. $N_{H_2O}/\tau_{100} = 10^8$ cm$^{-2}$ is adopted, corresponding to a constant H$_2$O abundance of 7.7 $\times 10^{-2}$ (Eq. (1)). Blue symbols indicate models with $\Delta V = 100$ km s$^{-1}$ and thus with variable $K_{vir}$ (Eq. (5)) indicated with the numbers. Green symbols show results with $\Delta V = 100 \times \tau_{100}$ km s$^{-1}$ simulating a constant value of $K_{vir} = 1.3$. When compared with observations, the modeled $L_2$ values should be considered a fraction of the observed IR luminosities (Sect. 4.3.1), and thus the modeled $L_2/L_{IR}$ values are upper limits.

Fig. 11. (a) Values of $N_{H_2O}$ for $\Delta V = 100$ km s$^{-1}$ as a function of $\tau_{100}$.
(b) $L_{H_2O}/L_{IR}$ as a function of $\tau_{100}$.
(c) $F_{25}/F_{60}$ as a function of $\tau_{100}$.
(d) $L_{adv}$ as a function of $\tau_{100}$.
(e) $F_{25}/F_{60}$ as a function of $\tau_{100}$.
Finally, we note that $T_{dust} = 75$ K would imply even shorter times scales and suggest high rates of ISM return from SNe and stellar winds. A follow-up study of the relationship between $L_{H2O}$ and $L_{HCN}$ is required to check this point. In addition, modeling the individual sources simultaneously in the continuum and the H$_2$O emission will provide further constraints on the nature of these regions.

5.2. Strong optically classified AGN sources

The general finding that the H$_2$O emission is similar in star-forming and strong-AGN sources (Y13) may simply indicate that the far-IR pumping of H$_2$O occurs regardless of whether the dust is heated via star formation or an AGN. There are, however, some differences between the two source types. Strong AGNs show a higher detection rate in H$_2$O $11_{00}$-00$_{11}$ (Y13), indicating that the gas densities are higher in the circumnuclear regions of AGNs. Another difference is that the $L_{H_2O}/L_{IR}$ ratios are somewhat lower in strong AGN sources (Y13). While relatively low columns of dust and H$_2$O in these sources could explain this observational result, it is also possible that high X-ray fluxes photodissociate H$_2$O, reducing its abundance relative to star-forming galaxies. High abundances of H$_2$O require effective shielding from UV and X-ray photons and thus high columns of dust and gas that, in AGN-dominated galaxies, may be effectively provided by an optically thick torus probably accompanied by starburst activity. In addition, warm dust further enhances $X_{H_2O}$ through an undepleted chemistry and pumps the excited H$_2$O levels, while warm gas will further boost $X_{H_2O}$ through reactions of OH with H$_2$. These appear to be the ideal conditions for the presence of large quantities of H$_2$O in the (circum)nuclear regions of galaxies.

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References

Appleton, P. N., Guillard, P., Boulaud, F., et al. 2013, ApJ, 777, 66
Bergen, E. A., Melnick, G. J., Staufer, J. R., et al. 2000, ApJ, 539, L129
Bothwell, M. S., Aguirre, J. E., Chapman, S. C., et al. 2013, ApJ, 779, 67
Bradford, C. M., Bolatto, A. D., Maloney, P. R., et al. 2011, ApJ, 741, L37
Bryant, P. M., & Scoville, N. Z. 1996, ApJ, 457, 678
Casey, C. M. 2012, MNRA, 425, 3094
Chabrier, G. 2003, ApJ, 586, L13
Combes, F., Rex, M., Rawle, T. D., et al. 2012, A&A, 538, L4
Dale, D. A., & Helou, G. 2002, ApJ, 576, 159
Daniel, P., Dubernet, M.-L., & Grosjean, A. 2011, A&A, 536, A76
Downes, D., & Eckart, A. 2007, A&A, 468, L57
Downes & Solomon, P. M. 1998, ApJ, 507, 615
Draine, B. T. 1985, ApJS, 57, 587
Dubernet, M.-L., Daniel, P., Grosjean, A., & Lin, C. Y. 2009, A&A, 497, 911
Dunne, L., Eales, S. A., & Edmunds, M. G. 2013, MNRA, 341, 589
Fischer, J., Luhman, M. L., Satyapal, S., et al. 1999, Ap&SS, 266, 91
Fischer, J., Sturm, E., González-Alfonso, E., et al. 2010, A&A, 518, L41
Gao, Y., & Solomon, P. M. 2004a, ApJ, 606, 271
Gao, Y., & Solomon, P. M. 2004b, ApJ, 152, 63
García-Burillo, S., Usero, A., Alonso-Herrero, A., et al. 2012, A&A, 539, A8
Goldsmith, P. F. 2001, ApJ, 557, 736
González-Alfonso, E., Smith, H. A., Fischer, J., & Cernicharo, J. 2004, ApJ, 613, 247
González-Alfonso, E., Smith, H. A., Ashby, M. L. N., et al. 2008, ApJ, 675, 303
González-Alfonso, E., Fischer, J., Isaak, K., et al. 2010, A&A, 518, L43
González-Alfonso, E., Fischer, J., Graciá-Carpio, J., et al. 2012, A&A, 541, A4 (G-A12)
González-Alfonso, E., Fischer, J., Bruderer, S., et al. 2013, A&A, 550, A25
González-Alfonso, E., Fischer, J., Graciá-Carpio, J., et al. 2014, A&A, 561, A27
Griffin, M. J., Abergel, A., Abreu, A., et al. 2010, A&A, 518, L3
Hailey-Dunsheath, S., Sturm, E., Fischer, J., et al. 2012, ApJ, 755, 712
Impellizzeri, C. M. V., McKean, J. P., Castangia, P., et al. 2008, Nature, 456, 927
Kovács, A., Omont, A., Beelen, A., et al. 2010, ApJ, 717, 29
Krips, M., Martin, S., Eckart, A., et al. 2011, ApJ, 736, 37
Lonsdale, C., Neufeld, D. A., Phillips, T. G., Gerin, M., & Neri, R. 2011, ApJ, 736, L6
Lupu, R. E., Scott, K. S., Aguirre, J. E., et al. 2012, ApJ, 757, 135
Meijerink, R., Kristensen, L. E., Weiß, A., et al. 2013, ApJ, 762, L16
Melnick, G. J., & Bergin, E. A. 2005, Adv. Space Res., 36, 1027
Müller, H. S. P., Thorwirth, S., Roth, D. A., & Winnewisser, G. 2001, A&A, 370, L49
Müller, H. S. P., Schlöder, F., Stutzki, J., & Winnewisser, G. 2005, J. Mol. Struct., 742, 215
Omont, A., Nerin, R., Cox, P., et al. 2011, A&A, 530, L3
Omont, A., Yang, C., Cox, P., et al. 2013, A&A, 551, A115 (O13)
Papadopoulos, P. P., & Seuqist, E. R. 1999, ApJ, 516, 114
Papadopoulos, P. P., Isaac, K. G., & van der Werf, P. P. 2007, ApJ, 668, 815
Perea-Santalla, M., Spinoglio, L., & Busquet, G., et al. 2013, ApJ, 768, 55
Pickett, H. M., Poynter, R. L., Cohen, E. A., et al. 1998, J. Quant. Spectr. Rad. Tran., 60, 883
Pilbratt, G. L., Riedinger, J. R., et al. 2013, ApJ, 779, 67
Poglitsch, A., Waelkens, C., Geis, N., et al. 2010, A&A, 518, L2
Preibisch, Th., Ossenkopf, V., Yorke, H.W., & Henning, Th. 1993, A&A, 279, 577
Rangwala, N., Maloney, P. R., Glenn, J., et al. 2011, ApJ, 743, 94
Riechers, D. A., Bradford, C. M., Clements, D. L., et al. 2013, Nature, 496, 329
Sakamoto, K., Wang, J., Wiedner, M. C., et al. 2008, ApJ, 684, 957
Snell, R. L., Howe, J. E., Ashby, M. L. N., et al. 2000, ApJ, 539, L101
Spilker, L., Pereira-Santalla, M., Busquet, G., et al. 2012, ApJ, 758, 1018
Snell, R. L., Howe, J. E., Ashby, M. L. N., et al. 2000, ApJ, 539, L129
van der Werf, P. P., Isaac, K. G., Meijerink, R., et al. 2010, A&A, 518, L42
van der Werf, P., Bricciano Alba, A., Spans, M., et al. 2011, ApJ, 741, L38
van Dishoeck, E. F., Kristensen, L. E., Benz, A. O., et al. 2011, PASP, 123,138
Yang C., Gao, Y., Omont, A., et al. 2013, ApJ, 771, L24 (Y13)
Arp 220 and NGC 1068 are prototypical sources that have been observed at essentially all wavelengths. With regard to their H$_2$O submm emission, these galaxies are extreme cases and deserve special consideration.

In the nearby ULIRG Arp 220, discrepancies between the observed SLED (Rangwala et al. 2011, Y13) and the single-component models of Figs. 3a1–c1 are worth noting. The observed high $L_d/L_{IR}$ $\approx$ 2.4 $\times$ 10$^{-5}$ (Fig. 8), together with the high 6/2 ratio of $\approx$1.4 (Fig. A.1a), suggest $T_{dust}$ $\gtrsim$ 65 K and $N_{H_2}$O $\gtrsim$ 10$^{17}$ cm$^{-2}$, consistent with detection of lines 7–8. However, high $T_{dust}$ and $N_{H_2}$O are mostly compatible with $F_d/F_3 >$ 1, while the observed ratio is $\approx$0.7 (Fig. A.1a). As in Mrk 231, a composite model is required to account for the H$_2$O SLED in this galaxy.

In sources with very optically thick and very warm cores such as Arp 220 (G-A12), the increase in $\tau_{100}$ above 1 decreases the submm H$_2$O fluxes due to the rise of submm extinction (Fig. 9). While higher $T_{dust}$ generates warmer SEDs, lowers the $L_d/L_{IR}$ ratios for lines 2–6, the increase in $\tau_{100}$ further decreases $L_d/L_{IR}$. This behavior suggests that the optimal environments for efficient H$_2$O submm line emission are regions with high far-IR radiation density but moderate extinction, i.e., those that surround the thick core(s) where the bulk of the continuum emission is generated. In contrast, the H$_2$O absorption at shorter wavelengths is more efficiently produced in the nearside layers of the optically thick cores, primarily if high-lying lines are involved. Absorption and emission lines are thus complementary, providing information on the source structure.

We have taken the models in G-A12 for Arp 220 to predict its submm H$_2$O emission. In Fig. A.1a, the blue symbols/line indicate the predicted H$_2$O fluxes towards the optically thick, warm nuclear region (both $C_{west}$ and $C_{east}$, see G-A12), indicating that most submm lines (with the exception of lines 3, 7, and 8) are predicted in absorption. The observed H$_2$O submm line emission (Rangwala et al. 2011) must therefore arise in the surrounding, optically thinner region, i.e., the $C_{extended}$ component, where the H$_2$O abundance in the inner parts ($R \approx$ 150 pc, where $T_{dust} = 70–90$ K) is increased relative to G-A12 (so $C_{extended}$ has $N_{H_2}$O $= 1.3 \times 10^{17}$ cm$^{-2}$ in Fig. A.1a). According to our model, the relatively low flux in line 4 is due to line absorption towards the nuclei. The main drawback of the model in Fig. A.1a is that line 7 is underestimated by a factor 2. The submm H$_2$O emission in Arp 220 traces a transition region between the compact optically thick cores and the extended kpc-scale disk (G-A12). The overall H$_2$O spectrum is, however, dominated by absorption of the continuum (Fig. A.1b).

Just the opposite set of conditions characterizes the nearby Seyfert 2 galaxy NGC 1068, since the nuclear continuum emission is optically thin and collisional excitation is important (S12). All detected H$_2$O lines, including those in the far-IR (100–200 $\mu$m) are seen in emission, and most of them show fluxes (in erg/s/cm$^2$) unrelated to wavelength, upper level energy (up to $\approx$1000 K), or A-Einstein coefficient (S12). In particular, the H$_2$O 2$_{21}$–1$_{10}$ (108 $\mu$m) and 2$_{21}$–2$_{12}$ (180 $\mu$m) lines share the same upper level and show similar fluxes but the A-Einstein coefficient of the 108 $\mu$m transition is a factor of 8.4 higher than that of the 180 $\mu$m transition. With pure collisional excitation, the only way to account for the observed line ratios is to invoke high densities and H$_2$O column densities, but also a relatively low $T_{gas}$ to avoid significantly populating the high-lying levels.
of continuum photons in the 322 H2O emission in NGC 1068 with lower densities and H2O sional excitation of the low-lying levels.

We have explored an alternative composite solution for the H2O emission in NGC 1068 with lower densities and H2O columns and higher Tgas, based on the far-IR pumping of the lines by an external anisotropic radiation field. In this framework, we can account for the weakness of the 108 μm line by the absorption of continuum photons, and indeed we would have to explain why this line is not observed to be even weaker than it is in absorption. The higher lying far-IR 322−311 emission line at 156.2 μm is in this scenario pumped through absorption of continuum photons in the 322−211 line at 90 μm.

For the first component, we closely follow H12 in modeling the moderate-excitation (ME) component as an ensemble of clumps, which are described by Tdust = 55 K, τ100 = 0.18, nH = 106 cm−3, Tgas = 150 K, and NH2O = 6.5 × 1016 cm−2, and Vturb = 15 km s−1 (giving Kvir ≈ 10, see H12). With a mass of 7.5 × 106 M⊙, this component is unable to account for the H2O submm lines 2−6, but generates a significant fraction of the observed emission in line 1 and some far-IR lines (Fig. A.2a and panel b).

We then added another, low-excitation (LE) component, which is identified with the gas generating the low-J CO lines (Krips et al. 2011, S12) and is thus assigned a density of nH = 2×104 cm−3. For simplicity, we also assume Tdust = 55 K, τ100 = 0.18, and NH2O = 6.5 × 1016 cm−2 as for the ME, but adopt the higher Vturb of 60 km s−1 (giving Kvir ≈ 7). For the LE component, and besides the internal far-IR field described by its Tdust and τ100, we also follow H12 in including an external field (associated with the emission from the whole region), which is described as a graybody with TBB = 55 K and τ100 = 0.05. The resulting mean specific intensity at 100 μm of the external field, Jext 100 μm, matches the value estimated by H12 within a factor of 2 (their Eq. (1)). A crucial aspect of the present approach is that this external field is assumed to be anisotropic, that is, it does not impinge into the LE clumps on the back side (in the direction of the observer). As a result, the external field contributes to the H2O excitation without generating absorption in the pumping far-IR lines (though some absorption is nevertheless produced by the internal field). As shown in Fig. A.2a, the LE component is expected to dominate the emission of the submm lines 2−6, as well as the emission of the majority of the far-IR lines. The required mass of the LE component is 3.5 × 107 M⊙, consistent with the mass inferred from the CO lines for the CND (S12), and the IR luminosity is 2.6 × 1010 L⊙.

A key assumption of the present model is that the external radiation field does not produce absorption in the far-IR lines, as otherwise (that is, in a perfectly isotropic radiation field) the strengths of the far-IR lines would weaken, and in particular, the H2O 221−110 line at 108 μm line would be predicted to be observed in absorption. The proposed anisotropy could be associated with the heating by the central AGN, and it seems possible as long as the source is optically thin in the far-IR. Radiative transfer in 3D would be required to check this feature. On the other hand, the external field, while having an important effect on the far-IR lines, has a secondary effect on the submm lines, which are primarily pumped by the internal (isotropic) radiation field (that is, by the dust that is mixed with H2O). With the caveat of the assumed intrinsic radiation anisotropy in mind, we preliminary favor this model over the pure collisional one in predicting the H2O submm fluxes and conclude that radiative pumping most likely plays an important role in exciting the H2O in the CND of NGC 1068.

From the models for these two very different sources and the case of Mrk 231 studied previously (G-A10), we conclude that the excitation of the submm H2O lines other than the 111−000 one is dominated by radiative pumping, though the relatively low-lying 202−111 line may still have a significant “collisional” contribution in some very warm/dense nuclear regions, and the radiative pumping may be enhanced with collisional excitation of the low-lying 111 and 212 levels. These individual cases also show that composite models to account for the full H2O far-IR/submm spectrum in a given source may be a rather general requirement.