

Herschel/PACS spectroscopy of NGC 4418 and Arp 220: H₂O, H₂¹⁸O, OH, ¹⁸OH, O_I, HCN, and NH₃^{*}

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ABSTRACT

Full range *Herschel*/PACS spectroscopy of the (ultra)luminous infrared galaxies NGC 4418 and Arp 220, observed as part of the SHINING key programme, reveals high excitation in H₂O, OH, HCN, and NH₃. In NGC 4418, absorption lines were detected with $E_{\text{lower}} > 800$ K (H₂O), 600 K (OH), 1075 K (HCN), and 600 K (NH₃), while in Arp 220 the excitation is somewhat lower. While outflow signatures in moderate excitation lines are seen in Arp 220 as have been seen in previous studies, in NGC 4418 the lines tracing its outer regions are redshifted relative to the nucleus, suggesting an inflow with $\dot{M} \lesssim 12 M_{\odot} \text{ yr}^{-1}$. Both galaxies have compact and warm ($T_{\text{dust}} \gtrsim 100$ K) nuclear continuum components, together with a more extended and colder component that is much more prominent and massive in Arp 220. A chemical dichotomy is found in both sources: on the one hand, the nuclear regions have high H₂O abundances, $\sim 10^{-5}$, and high HCN/H₂O and HCN/NH₃ column density ratios of 0.1–0.4 and 2–5, respectively, indicating a chemistry typical of evolved hot cores where grain mantle evaporation has occurred. On the other hand, the high OH abundance, with OH/H₂O ratios of ~ 0.5 , indicates the effects of X-rays and/or cosmic rays. The nuclear media have high surface brightnesses ($\gtrsim 10^{13} L_{\odot}/\text{kpc}^2$) and are estimated to be very thick ($N_{\text{H}} \gtrsim 10^{25} \text{ cm}^{-2}$). While NGC 4418 shows weak absorption in H₂¹⁸O and ¹⁸OH, with a ¹⁶O-to-¹⁸O ratio of $\gtrsim 250$ –500, the relatively strong absorption of the rare isotopologues in Arp 220 indicates ¹⁸O enhancement, with ¹⁶O-to-¹⁸O of 70–130. Further away from the nuclear regions, the H₂O abundance decreases to $\lesssim 10^{-7}$ and the OH/H₂O ratio is reversed relative to the nuclear region to 2.5–10. Despite the different scales and morphologies of NGC 4418, Arp 220, and Mrk 231, preliminary evidence is found for an evolutionary sequence from infall, hot-core like chemistry, and solar oxygen isotope ratio to high velocity outflow, disruption of the hot core chemistry and cumulative high mass stellar processing of ¹⁸O.

Key words. galaxies: ISM – line: formation – ISM: kinematics and dynamics – infrared: galaxies – submillimeter: galaxies

1. Introduction

From the first CO observations of IRAS galaxies (Young et al. 1984), much effort has been devoted to understanding spectroscopic observations of molecules in (ultra)luminous infrared galaxies ((U)LIRGs), and how they are related to the conditions traced by the continuum and line observations of atoms and ions. The launch of the Infrared Space Observatory (ISO) and, more recently, the *Herschel* Space Observatory, have opened a new window to study extragalactic sources in the far-infrared (hereafter, far-IR) domain, where the bulk of the (U)LIRG luminosity is emitted. The relevance of far-IR molecular spectroscopy of (U)LIRGs is well illustrated with the initial ISO result of Fischer et al. (1999), that the fine-structure lines of atoms and ions

decrease in strength, as absorption in molecular lines, specifically H₂O and OH, increase in depth.

Water (H₂O) and hydroxyl (OH) are indeed key molecular species that trace relevant physical and chemical properties of the interstellar medium in luminous infrared extragalactic sources. Powerful OH mega-masers are common in ULIRGs, and H₂O masers are found in AGN accretion disks and in post-shocked gas associated with nuclear jets (see Lo 2005, for a review). With many transitions lying at far-IR wavelengths, where the bulk of the luminosity is emitted, H₂O and OH are mainly excited through absorption of far-IR photons (González-Alfonso et al. 2004, hereafter G-A04), and thus their excitation helps probe the general properties of the underlying far-IR continuum sources (González-Alfonso et al. 2008). Chemically, H₂O is expected to trace an undepleted chemistry where grain mantles are evaporated; both H₂O and OH are also boosted in shocks and, especially OH, in X-ray and cosmic ray dominated regions (XDRs and CRDRs). Furthermore, OH has turned out to be

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a unique tracer of massive molecular outflows (Fischer et al. 2010; Sturm et al. 2011). Recently, H₂O has been detected in 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), and thus understanding its role in the local Universe will be crucial for future routine observations of H₂O with ALMA in the far Universe. HCN is another key molecule widely studied in local (U)LIRGs at (sub)millimeter wavelengths (e.g., Aalto et al. 1995). NH₃, first detected in extragalactic sources by Martin & Ho (1979), is another important tracer; in Arp 220, it was detected at far-IR wavelengths with ISO (G-A04) and at centimeter wavelengths by Takano et al. (2005) and recently by Ott et al. (2011). With its high sensitivity and spectral resolution at far-IR wavelengths, the *Herschel*/PACS instrument (Pilbratt et al. 2010; Poglitsch et al. 2010) provides new opportunities for using the far-IR transitions of these molecules to probe the kinematic, chemical, and radiative activity in IR luminous galaxies.

We report in this work *Herschel*/PACS spectroscopic observations of H₂O, OH, their ¹⁸O isotopologues, NH₃, and the surprising detection of highly excited HCN, in NGC 4418 and Arp 220. NGC 4418 is a peculiar, single nucleus galaxy, with a moderate luminosity ($\sim 10^{11} L_{\odot}$) but with other properties similar to warm ULIRGs: a high $L_{\text{FIR}}/M_{\text{H}_2}$ ratio and an extreme [C II] deficit (e.g. Graciá-Carpio et al. 2011), a high continuum surface brightness, an extremely compact luminosity source (Evans et al. 2003), and warm infrared colors ($S_{25 \mu\text{m}}/S_{60 \mu\text{m}} = 0.23$, $S_{60 \mu\text{m}}/S_{100 \mu\text{m}} = 1.37$). We adopt a distance to the source of 29 Mpc. Arp 220 is the prototypical and nearest ULIRG, showing a double nucleus and a luminosity of $\approx 1.3 \times 10^{12} L_{\odot}$. We adopt a distance to the source of 72 Mpc. The observations are described in Sect. 2; models are shown in Sect. 3; model results are discussed in Sect. 4, and our main conclusions are summarized in Sect. 5.

2. Observations and results

2.1. Observations

The full (52.3–98, 104.6–196 μm), high resolution, PACS spectra of NGC 4418 and Arp 220, taken as part of the guaranteed-time key programme SHINING, were observed on July 27th and February 27th (2010), respectively. The spectra were taken in high spectral sampling density mode using first and second orders of the grating. The velocity resolution of PACS in first order ranges from $\approx 320 \text{ km s}^{-1}$ at 105 μm to $\approx 180 \text{ km s}^{-1}$ at 190 μm , and in second order from $\approx 210 \text{ km s}^{-1}$ at 52 μm to $\approx 110 \text{ km s}^{-1}$ at 98 microns. For NGC 4418, we also present a scan around the [O I] 63 μm line taken in third order with velocity resolution of $\approx 85 \text{ km s}^{-1}$. The data reduction was mostly done using the standard PACS reduction and calibration pipeline (ipipe) included in HIPE 5.0 975. The reduction of Arp 220 required, however, two additional steps in order to correct for pointing errors that resulted in significant variations of the continuum level of the central spaxel¹ as well as in wavelength offsets generated by pointing errors along the dispersion direction of the slit (Poglitsch et al. 2010). These effects were produced by the movement of the source between the central spaxel and a neighboring spaxel. In order to correct for them, (i) the emission from the two spaxels with highest signal were added together in an intermediate step in the pipeline, which significantly improved the continuum baseline of the combined spectrum but increased the noise by a

¹ PACS has 5×5 spatial pixels (spaxels), each with $9'' \times 9''$ resolution and covering a field of $47'' \times 47''$ (Poglitsch et al. 2010).

factor² $\approx \sqrt{2}$; (ii) the time evolution of the pointing shifts was reconstructed from the star tracker frames, and wavelength calibration was corrected according to Fig. 8 by Poglitsch et al. (2010). Pointing errors across the slit were found from 0 to $\sim 3''$, resulting in velocity shifts of $\leq 60 \text{ km s}^{-1}$. We estimate that the associated uncertainties are below 30 km s^{-1} , though they may be higher for some individual lines.

For the final calibration, the spectrum was normalized to the telescope flux and recalibrated with a reference telescope spectrum obtained from observations of Neptune. The flux density of the spectrum in the central spaxel(s) was then rescaled to the value of the total continuum of the source obtained by the combination of the 25 spaxels of the PACS spectrometer. This method assumes that the distribution of the IR continuum and the lines are similar for the spatial resolution of the observations. Indeed the line to continuum ratio in the central and the combined 25 spaxels was found to be the same for all strong lines except for the ground-state OH 119 and 79 μm in Arp 220, which display 9% and 3% deeper absorption in the central spaxels. The latter OH lines thus appear to show low-level reemission (probably through scattering) over kpc spatial scales. In general, the comparison indicates that both sources are at far-IR wavelengths point-sources compared with the PACS $9'' \times 9''$ spatial resolution ($\sim 1.3 \times 1.3 \text{ kpc}^2$ for NGC 4418 and $\sim 3.1 \times 3.1 \text{ kpc}^2$ for Arp 220).

The continua of both sources are shown in Fig. 1, including the *Spitzer* IRS spectra (Spoon et al. 2007); the models are discussed in Sect. 3. Both galaxies show strong silicate absorption at 9.7 μm , with PAH emission that is weak in Arp 220 and only weakly detected at 11.2 μm in NGC 4418 (Spoon et al. 2007). Besides the obvious differences in luminosity, a striking contrast between both sources is the $S_{60 \mu\text{m}}/S_{25 \mu\text{m}}$ ratio, which is ≈ 4 in NGC 4418 and approaches ≈ 13 in Arp 220. The higher value in Arp 220 indicates that larger amounts of dust surround the nuclei in an extended region (ER in G-A04, denoted here as C_{extended}), both extinguishing the nuclear emission at 25 μm and contributing to the far-IR continuum. This emission can be interpreted as heating of dust by the radiation emanating from the nuclei (Soifer et al. 1999, G-A04). In NGC 4418, the warmer spectral energy distribution (SED) suggests that the amount of dust in C_{extended} is lower, but still probably significant (see Sect. 3). On the other hand, the (sub)millimeter emission in Arp 220 is dominated by the nuclei as revealed by interferometric (sub)millimeter observations (Downes & Eckart 2007; Sakamoto et al. 2008), indicating extreme opacities in, and high luminosities from the nuclei. No interferometric observations are available for NGC 4418.

Spectroscopic data used for both line identification and radiative transfer modeling were taken from the JPL (Pickett et al. 1998) and CDMS (Müller et al. 2001, 2005) catalogues. Figure 2 shows the energy level diagrams of OH and H₂O. The spectra around the H₂O lines are shown in Fig. 3 (blue and green bands, $\lambda < 100 \mu\text{m}$) and Fig. 4 (red band, $\lambda > 100 \mu\text{m}$), while high-lying H₂O lines tentatively detected in NGC 4418 (blue-dashed arrows in Fig. 2) are shown in Fig. 5. The OH line profiles are presented in Fig. 6. Figures 7 and 8 show excerpts of the PACS spectra around the H₂¹⁸O and ¹⁸OH lines, respectively. The HCN and NH₃ lines are displayed in Figs. 9 and 10, respectively. Figure 11 compares the line profiles of the [O I] 63 and 145 μm transitions with those of some OH lines. Figure 12 compares the

² Since the neighboring spaxel has a signal much lower than the central one, the subsequent final calibration leaves the factor $\sqrt{2}$ nearly unchanged.

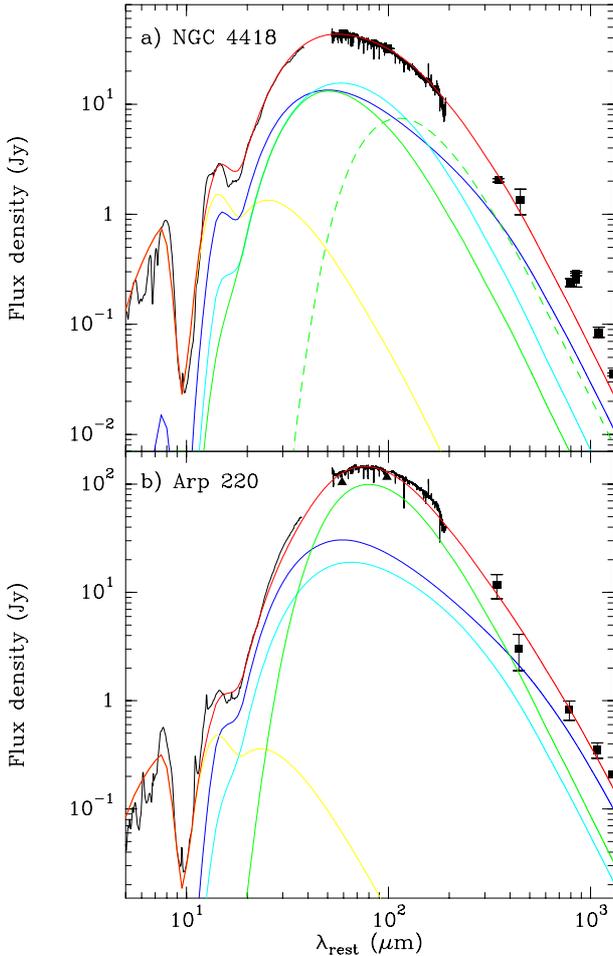


Fig. 1. Spectral energy distribution of NGC 4418 and Arp 220 from mid-IR to millimeter wavelengths. Both the *Herschel*/PACS and the *Spitzer*/IRS spectra are shown. Data points at (sub)millimeter wavelengths for NGC 4418 are from (Yang & Phillips 2007, 350 μm), (Roche & Chandler 1993, 450, 800, and 1100 μm), (Dunne et al. 2000; Lisenfeld et al. 2000, 850 μm), and (Albrecht et al. 2007, 1300 μm). For Arp 220, they are taken from (Eales et al. 1989, 450 μm); (Rigopoulou et al. 1996, 350, 800, and 1100 μm); and (Sakamoto et al. 1999, 2008, 1300 μm). Models discussed in Sect. 3 are included. For NGC 4418, the yellow, blue, light-blue, and solid-green curves show the models for the hot, core, warm, and extended components, respectively, with parameters given in Table 1. An additional cold component, shown with the dashed-green curve, is included to better fit the SED at long wavelengths. For Arp 220, the yellow, blue, light-blue, and solid-green curves show the models for the hot, western nucleus, eastern nucleus, and extended components, respectively (Table 1).

line shapes of two HCO^+ transitions observed with high spatial resolution by Sakamoto et al. (2009) in Arp 220, with selected lines observed with *Herschel*/PACS. Results of the continuum and line modeling are summarized in Tables 1 and 2, and the line equivalent widths of the H_2O , $[\text{O I}]$ and OH, HCN, NH_3 , H_2^{18}O , and ^{18}OH lines are listed in Tables 3 to 8.

2.2. Systemic redshifts

Line parameters were derived by subtracting baselines and fitting Gaussian curves to all spectral features. One relevant question in our study is the zero-velocity adopted for the high-excitation molecular gas in the nuclear region of the galaxies. In NGC 4418, the excited H_2O lines do not show any evidence

of systematic shifts indicative of outflowing or inflowing gas. Figure 13 indicates that the only H_2O line clearly redshifted relative to all others is the ground-state $2_{12} \rightarrow 1_{01}$ at 179.5 μm , which is expected to be contaminated by CH^+ (2–1) (see below). From all other H_2O lines, the average redshift is $z = 0.007035 \pm 0.000070$ ($cz = (2110 \pm 20) \text{ km s}^{-1}$), where the error denotes the standard deviation of the mean. The inferred redshift is fully consistent with observations of CO, CN, HNC, and other molecular species observed at millimeter wavelengths (e.g. Aalto et al. 2007a). The Sloan Digital Sky Survey (SDSS) spectrum of NGC 4418 also gives a consistent redshift for the optical absorption/emission lines of $z = 0.0070$ and 0.0072, respectively (D. Rupke, private communication). Finally, this is also consistent with the redshift measured for the high-lying OH lines (see below), which also trace the nuclear component, and with that of the $[\text{C II}]$ emission line at 157.741 μm , $z = 0.007050$, which we adopt as the reference value. In Arp 220, Sakamoto et al. (2009) detected P-Cygni profiles in excited submillimeter lines of HCO^+ toward both nuclei, indicating dense outflowing gas in the nuclei (see also Fig. 12 and Sect. 2.7). The transition from absorption to emission occurs at a velocity of $\approx 5420 \text{ km s}^{-1}$ toward both nuclei, which we adopt as the systemic redshift ($z = 0.0181$). The foreground absorption traced by CO (3–2) toward the western nucleus lies at a lower velocity, $\approx 5350 \text{ km s}^{-1}$. The line velocity shifts (V_{shift}) relative to the above systemic redshifts, the line widths, and the equivalent widths (W_{eq}) are plotted in Fig. 13 for the H_2O lines and in Fig. 14 for the OH lines.

2.3. H_2O and OH

Based on the H_2O spectra and the molecular line positions shown in Figs. 3 and 4, most H_2O lines are free of contamination from lines of other species, with the following exceptions: as mentioned above, the H_2O $2_{12} \rightarrow 1_{01}$ line in Fig. 4q at 179.5 μm is blended with CH^+ ; the $8_{08} \rightarrow 7_{17}$ line in Fig. 3f is blended with highly excited NH_3 (see Fig. 10a); the $5_{24} \rightarrow 4_{13}$ (Fig. 3i) and the $2_{21} \rightarrow 2_{12}$ lines (Fig. 4q) may have some contribution from CH; finally, the spectral feature at 104 μm associated in Fig. 4a with the $6_{15} \rightarrow 6_{06}$ line is probably contaminated by OH^+ . Other contaminated lines marked with dashed-green arrows in Fig. 2 are not shown. The OH lines in Fig. 6 have relatively weak contamination by NH_3 in the red Λ -component of the 84 μm doublet (panel e, see Fig. 10c), and by H_2O in the blue Λ -component of the 65 μm doublet (panel f).

The detections summarized in Fig. 2 indicate extreme excitation in the nuclei of both galaxies. In Arp 220, lines with lower level energy up to $E_{\text{lower}} \approx 600 \text{ K}$ in both H_2O ($7_{07} \rightarrow 6_{16}$ and $7_{17} \rightarrow 6_{06}$, Fig. 3j, the latter contaminated by excited NH_3) and OH ($\Pi_{1/2}9/2 \rightarrow 7/2$, Fig. 6i) are detected. NGC 4418 shows even higher-lying lines, with detected H_2O lines as high as $8_{18} \rightarrow 7_{07}$ and $7_{16} \rightarrow 6_{25}$ (Figs. 3f, g; $E_{\text{lower}} \gtrsim 800 \text{ K}$). These are the highest-lying H_2O lines detected in an extragalactic source to date.

The relative strengths of the H_2O and OH lines in NGC 4418 and Arp 220 show a striking dependence on E_{lower} . The lowest-lying ($E_{\text{lower}} \lesssim 200 \text{ K}$) H_2O lines, especially the $2_{12} \rightarrow 1_{01}$ transition at 179.5 μm (Fig. 4q), are stronger in Arp 220 than in NGC 4418, but higher-lying lines are stronger in NGC 4418 (see Fig. 13). The effect is even more clearly seen in OH (Fig. 14), where the ground-state lines (upper row in Fig. 6) are much stronger in Arp 220, the intermediate $\Pi_{3/2}5/2 \rightarrow 3/2$ transitions at 84 μm (Fig. 6e) have similar strengths, and higher excited OH lines (Figs. 6f–i) are stronger in NGC 4418. This is partially a consequence of the C_{extended} component in Arp 220: since W_{eq}

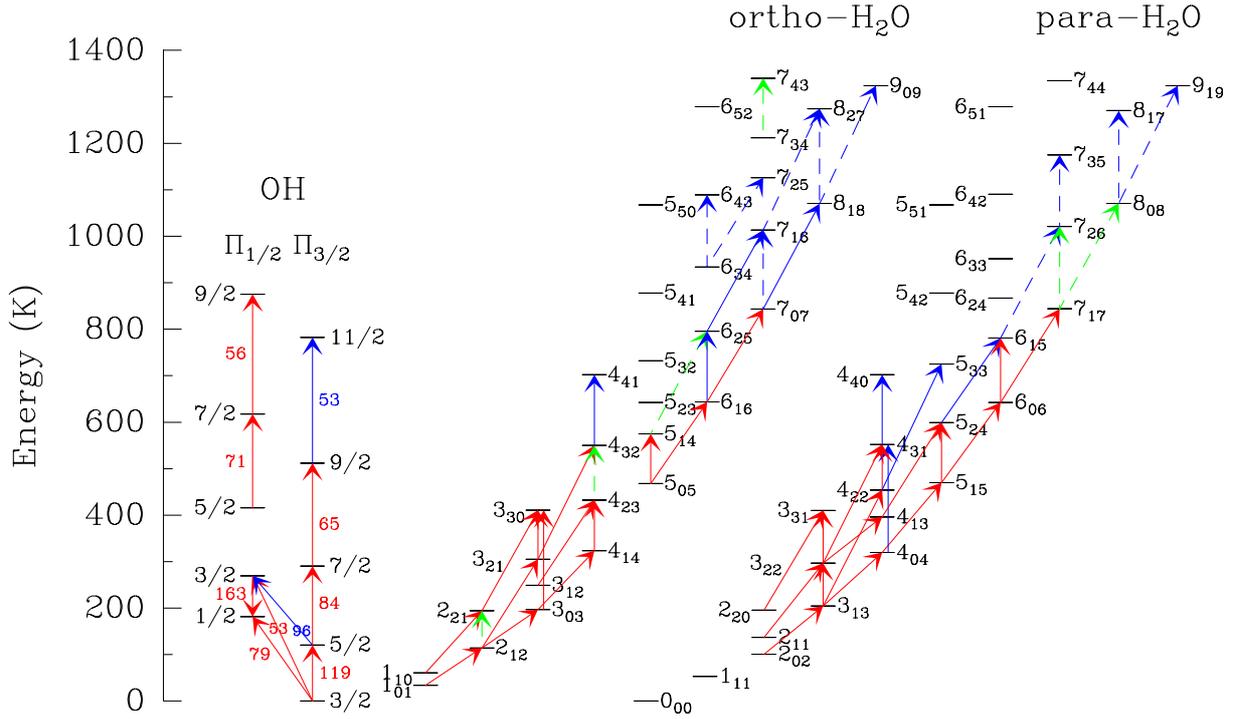


Fig. 2. Energy level diagrams of OH and H₂O (ortho and para). Red arrows indicate lines detected in both sources; blue arrows denote lines detected only in NGC 4418, green-dashed arrows mark transitions contaminated (blended) by lines of other species, and blue-dashed arrows denote marginal detections in NGC 4418. The small numbers in the OH diagram indicate rounded wavelengths in μm .

are calculated relative to the observed (nuclear+ C_{extended}) continuum, the high-lying lines arising from the nuclei are reduced due to the contribution by C_{extended} to the continuum, which is more prominent in Arp 220. In other words, the high-lying lines are more continuum-diluted in Arp 220 than in the relatively “naked” NGC 4418, which is consistent with the continuum models shown in Sect. 3. On the other hand, C_{extended} in Arp 220 produces strong absorption in the low-lying lines, thus increasing their W_{eq} relative to that in NGC 4418.

Nevertheless, dilution in the continuum cannot explain the higher excitation indicated by the very high-lying lines of H₂O and OH in NGC 4418. This is best seen in Figs. 13g, h, where the line fluxes are normalized relative to that of the excited $3_{30} \rightarrow 2_{21}$ H₂O line at 66.4 μm . The latter line (Fig. 3g) is well detected in both sources and, with $E_{\text{lower}} = 160$ K, is not expected to be significantly contaminated by absorption of extended low-excitation H₂O in Arp 220. Lines with E_{lower} above 500 K are shown to produce, relative to $3_{30} \rightarrow 2_{21}$, more absorption in NGC 4418 than in Arp 220. Also, as mentioned above, the H₂O $8_{18} \rightarrow 7_{07}$ and $7_{16} \rightarrow 6_{25}$ transitions (Figs. 3f, g) are only detected in NGC 4418 (the $8_{08} \rightarrow 7_{17}$ line in Fig. 3f is contaminated by NH₃, and the feature is not detected in Arp 220). Two more para-H₂O transitions detected only in NGC 4418 are the $5_{33} \rightarrow 4_{22}$ and $4_{40} \rightarrow 4_{31}$ lines (Figs. 3a, r); the lower levels of these lines are non-backbone and thus require high columns to be significantly populated. Other H₂O lines detected only in NGC 4418 are the $6_{25} \rightarrow 6_{16}$ and $4_{41} \rightarrow 4_{32}$ at 94.7 μm , but the Arp 220 spectrum at this wavelength shows a very broad feature, possibly due to pointing or instrumental effects (Fig. 3q).

The spectrum of NGC 4418 clearly shows two intrinsically weak H₂O lines with $\Delta K_{\pm 1} = \pm 3$, the $4_{31} \rightarrow 4_{04}$ line at 61.8 μm and the $3_{30} \rightarrow 3_{03}$ line at 67.3 μm (Figs. 3e, h). All other detected H₂O lines have higher transition probabilities and, with the exception of the very high-lying lines, are expected to be strongly

saturated. While the ortho-H₂O 67.3 μm line is also detected in Arp 220 within a wing-like feature that probably has some contribution from H₂¹⁸O $3_{30} \rightarrow 2_{21}$, the para-H₂O 61.8 μm line is not detected in Arp 220. The high columns in NGC 4418 are also confirmed by comparing the absorption in the ortho/para pair $4_{41} \rightarrow 4_{32}$ and $4_{40} \rightarrow 4_{31}$ (Figs. 3q, r), which have similar lower level energies (≈ 550 K), wavelengths, and transition probabilities ($A \approx 0.15$ s⁻¹). For an ortho-to-para ratio of 3, one would expect the same ratio of 3 for W_{eq} in the optically thin regime, but this is as low as 1.15 indicating that both lines are still well saturated.

Even higher-excitation lines of H₂O, with $E_{\text{lower}} \approx 900$ –1100 K, may be present in the spectrum of NGC 4418 (blue-dashed arrows in Fig. 2). Among these features, shown in Fig. 5, the most likely detection is the $7_{26} \rightarrow 6_{15}$ line in Fig. 5c, all other features being marginal. In particular, the 92.8 μm feature in (f) has a non-Gaussian shape. Nevertheless, all features together appear to indicate more extreme excitation in the nucleus of NGC 4418. This is plausible, as HCN rotational lines with $E_{\text{lower}} \geq 1075$ K are detected in NGC 4418 (see below).

As discussed earlier, dilution in the continuum also lowers the W_{eq} of the high-lying OH lines in Arp 220 relative to the values in NGC 4418; however, the most excited OH transitions, the $\Pi_{1/2}$ $9/2 \rightarrow 7/2$ and $\Pi_{1/2}$ $11/2 \rightarrow 9/2$ lines at 56 and 53 μm , respectively, are intrinsically stronger in NGC 4418 according to our decomposition of the continuum. Another effect of C_{extended} is also worth noting: the only OH transition observed in emission above the continuum, the $\Pi_{1/2}$ $3/2 \rightarrow 1/2$ doublet at 163 μm , is excited through absorption of continuum photons in the 35 and 53.3 μm doublets followed by a cascade down to the ground OH state (see Appendix II by Genzel et al. 1985), and is therefore expected to arise in the C_{extended} component (G-A04). The strong OH 163 μm emission in Arp 220 reflects the massive envelope around its nuclei. In NGC 4418, the doublet is weaker

but still in emission, also hinting at the existence of a C_{extended} component around its nucleus.

2.4. H_2^{18}O and ^{18}OH

The spectra around relevant H_2^{18}O and ^{18}OH transitions in NGC 4418 and Arp 220 are displayed in Figs. 7 and 8. Close spectral features due to H_3O^+ , NH_2 , C_3 , and CH^+ are also indicated. H_2^{18}O is detected in both sources, though in relatively low-lying lines. The highest-lying detected line is the $4_{32} \rightarrow 3_{21}$ transition with $E_{\text{lower}} \approx 270$ K in Fig. 7a, as detection of the $6_{16} \rightarrow 5_{05}$ transition in panel e is rather marginal. The most striking feature in Fig. 7 is the relative amount of absorption observed in NGC 4418 and Arp 220. While the absorption in the main isotopologues is stronger in NGC 4418 than in Arp 220 (Figs. 3 and 4), the opposite behavior is generally found for the absorption in the rare isotopologues. This is best seen in the $3_{31} \rightarrow 2_{20}$, $3_{21} \rightarrow 2_{12}$, $2_{21} \rightarrow 1_{10}$ (showing redshifted emission in Arp 220), $3_{13} \rightarrow 2_{02}$, and $2_{21} \rightarrow 2_{12}$ lines. There are, however, two spectral features nearly coincident with the $4_{23} \rightarrow 3_{12}$ and $4_{14} \rightarrow 3_{03}$ H_2^{18}O lines at 79.5 and 114.3 μm (panels d and h, respectively), with absorption in NGC 4418 apparently stronger than in Arp 220, but the latter is subject to an uncertain baseline.

The ^{18}OH lines in Fig. 8, specifically the ^{18}OH 85 and 120 μm doublets, confirm the ^{18}O enhancement in Arp 220. The blueshifted Λ -component of the ^{18}OH 120 μm doublet is strongly contaminated by $\text{CH}^+ J = 3 \rightarrow 2$ in both sources, but the uncontaminated redshifted Λ -component, undetected in NGC 4418, is strong in Arp 220. It is also worth noting that the two ^{18}OH 85 μm Λ -components show rather different absorption depths in Arp 220. This Λ -asymmetry is not expected to arise from radiative pumping or opacity effects, because the Λ -components of any transition have the same radiative transition probabilities, and the corresponding lower levels tend to be equally populated. Indeed, the absorption in the corresponding Λ -components of the main isotopologue at 84 μm are very similar (Fig. 6e). The ^{18}OH 85 μm Λ -asymmetry in Arp 220 is further discussed in Sect. 3.2.3. The ^{18}OH Λ -component at 65.54 μm in Fig. 8a is partially blended with two lines of NH_2 and, together with the expected contribution by H_2O^+ at 65.61 μm , form a broad feature with uncertain baseline. The red Λ -component at 65.69 μm appears to be stronger in Arp 220 than in NGC 4418.

2.5. HCN

HCN is a key molecule widely studied in both Galactic and extragalactic sources. In NGC 4418 and Arp 220, the low-lying lines at millimeter wavelengths have been observed by Aalto et al. (2007a,b) and Wiedner et al. (2004). The $\nu_2 = 1^1$ vibration-rotation band at 14 μm was detected in both sources by Lahuis et al. (2007), and rotational emission from the upper vibrational state in NGC 4418 has been detected by Sakamoto et al. (2010). The $\nu_2 = 1^1$ l-type HCN lines from $J = 4-6$ at centimeter wavelengths were detected in absorption toward Arp 220 (Salter et al. 2008). Among the 15 extragalactic sources detected in the HCN band, the Lahuis et al. (2007) analysis indicated that NGC 4418 has the second highest HCN column. Recently, Rangwala et al. (2011) have reported the detection of several emission/absorption HCN lines with *Herschel*/SPIRE in Arp 220.

We report in Fig. 9 the PACS detection of HCN absorption in pure rotational transitions at far-IR wavelengths in both NGC 4418 and Arp 220. In NGC 4418, all transitions from

$J = 18 \rightarrow 17$ ($E_{\text{lower}} = 650$ K) to $J = 23 \rightarrow 22$ ($E_{\text{lower}} = 1075$ K) are clearly identified. Furthermore, there are hints of absorption up to the $J = 25 \rightarrow 24$ transition ($E_{\text{lower}} = 1275$ K). In Arp 220, the $J = 20 \rightarrow 19$ line is clearly contaminated by H_3O^+ and NH_2 , and the $J = 23 \rightarrow 22$ one by C_3 and possibly also by NH_2 . The $J = 19 \rightarrow 18$ line is weak, suggesting that this transition is tracing the tail of the Spectral Line Energy Distribution (SLED). However, a clear feature is found at the wavelength of the $J = 21 \rightarrow 20$ line, and the $J = 22 \rightarrow 21$ line could show some marginal absorption as well. Nevertheless, we consider the identification of the $J = 21 \rightarrow 20$ line as questionable given the weakness of the nearby rotational HCN lines and the possible contamination by other species.

Fluxes derived from Gaussian fits are shown in Fig. 15 as a function of E_{lower} , where values derived from *Herschel*/Spire observations by Rangwala et al. (2011) are included for Arp 220. The HCN excitation in NGC 4418 is extreme, with the SLED apparently peaking at $J = 21 \rightarrow 20$ ($E_{\text{lower}} \approx 900$ K). The striking characteristic of the far-IR HCN lines is that they are detected in absorption against the far-IR continuum, indicating that the dust temperature and far-IR continuum opacities behind the observed HCN are high; otherwise the lines would be detected in emission. We argue in Sect. 3 that the H_2O , OH , and HCN lines in NGC 4418 are tracing a high luminosity, compact nuclear source, denoted as the *nuclear core* (C_{core}). In Arp 220, the HCN SLED as seen by *Herschel*/Spire (Rangwala et al. 2011) peaks at $J = 16 \rightarrow 15$ ($E_{\text{lower}} \approx 500$ K) indicating, like H_2O , more moderate excitation, but a second, higher-excitation component could be present if the 161.3 μm spectral feature is due to HCN $J = 21 \rightarrow 20$. As shown in Sects. 3.2.4 and 3.4.1, high HCN columns are required to explain the data.

2.6. NH_3

Ammonia is another N-bearing species widely observed in Galactic sources mostly through the pure-inversion transitions from metastable ($J = K$) levels at centimeter wavelengths (see Ho & Townes 1983, for a review). The rotation-inversion transitions lie at far-IR wavelengths, and many of them have been detected with ISO toward Sgr B2 (Ceccarelli et al. 2002; Polehampton et al. 2007) indicating a hot, low dense molecular layer interpreted in terms of shock conditions (Ceccarelli et al. 2002). Detections of far-IR NH_3 lines in extragalactic sources were presented, together with a preliminary analysis, by G-A04 in Arp 220. In Fig. 10 we show the *Herschel*/PACS detection of high-excitation, far-IR NH_3 lines in both NGC 4418 and Arp 220.

NH_3 has two species, ortho- NH_3 ($K = 3n$) and para- NH_3 ($K \neq 3n$), with an expected ortho-to-para abundance ratio of unity (Umehoto et al. 1999). All rotational (J, K) levels, except those of the $K = 0$ ladder, are split into 2 inversion doubling sublevels (a for asymmetric and s for symmetric), which for a given J have decreasing level energy with increasing K . Radiative transitions are only allowed within K -ladders, thus only collisions can populate the $K > 1$ ladders and the absorption from different K -ladders is then sensitive to the gas temperature. Within a given K -ladder, both collisions and absorption of far-IR photons can pump the $J > K$ non-metastable levels. Since the $a \rightarrow s$ ($s \rightarrow a$) $J + 1 \rightarrow J$ transitions of different K -ladders have similar wavelengths, the lines are crowded in wavelength and overlapping in some cases, with severe blending between the $K = 0$ and $K = 1$ ladders. The PACS domain covers the range from the $(3, K)a \rightarrow (2, K)s$ (≈ 170 μm , Fig. 10g)

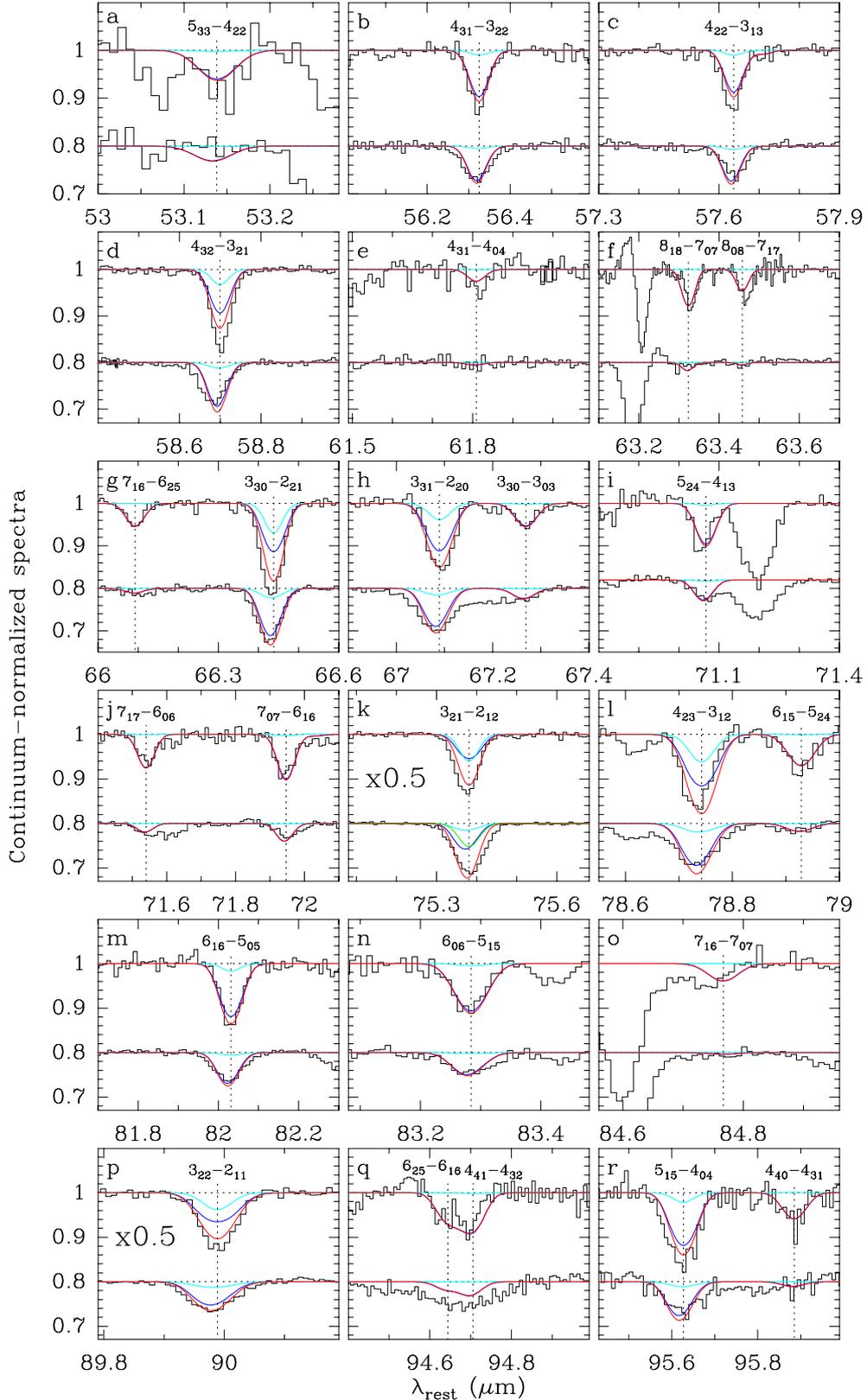


Fig. 3. H₂O lines in the blue and green bands ($\lambda < 100 \mu\text{m}$) detected in NGC 4418 (upper spectra in each panel) and Arp 220 (lower spectra). The spectra, histograms with black solid lines, have been scaled by a factor of 0.5 in panels **k**) and **p**). Vertical dotted lines indicate the rest wavelengths of the lines relative to $z = 0.00705$ and 0.0181 for NGC 4418 and Arp 220, respectively. Model results are also shown. For NGC 4418, the blue and light-blue curves show the models for the C_{core} and C_{warm} components, respectively; for Arp 220, the blue and light-blue lines show the estimated contributions from C_{west} and C_{east} , and the green curve (in panel **k**) shows the contribution by C_{extended} . Red is total. Model parameters are given in Tables 1 and 2.

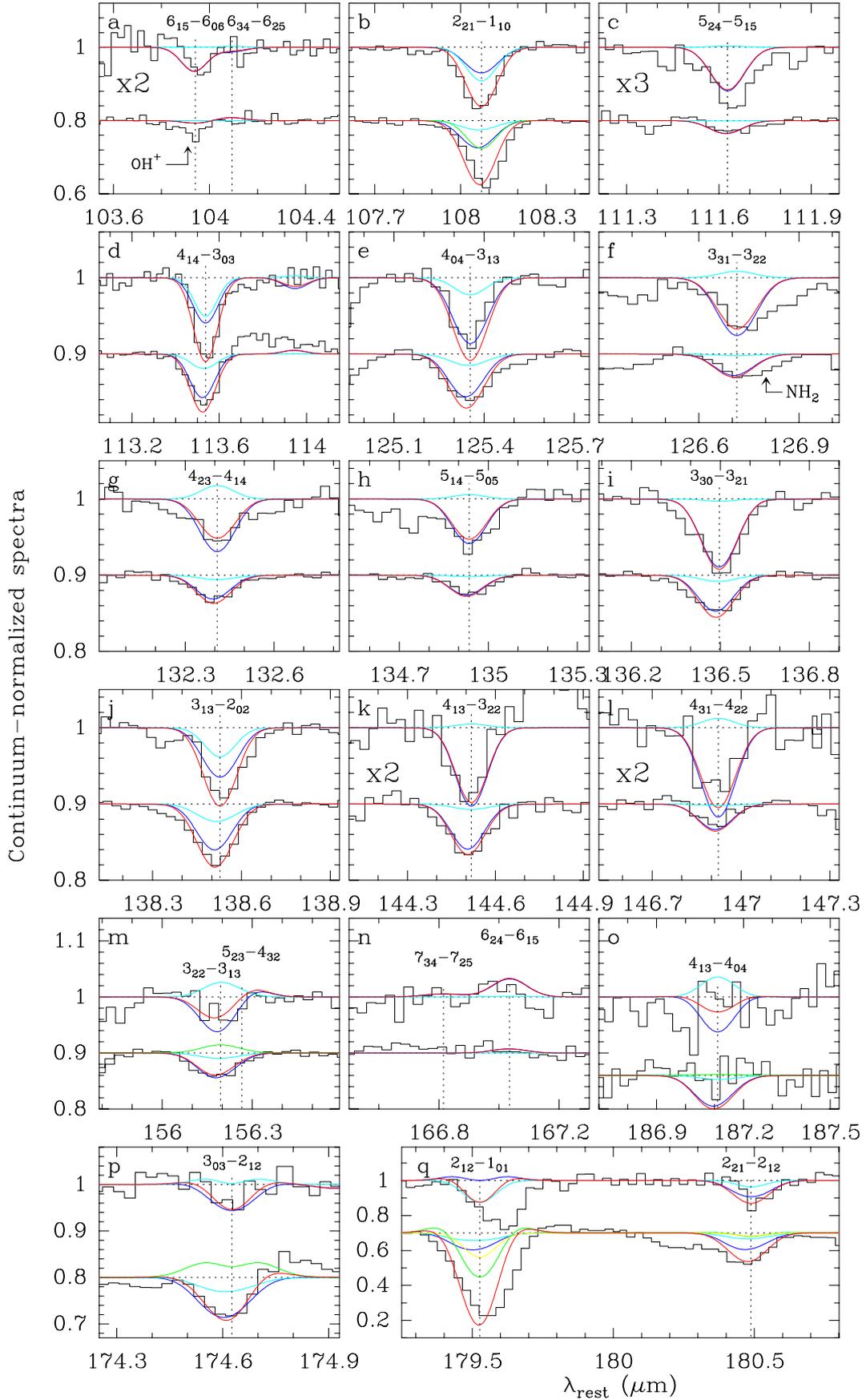


Fig. 4. H₂O lines in the red band ($\lambda > 100 \mu\text{m}$) detected in NGC 4418 (upper spectra in each panel) and Arp 220 (lower spectra). The spectra have been scaled by a factor of 2 in panels **a**), **k**) and **l**), and by 3 in panel **c**). Model results are also shown. Color codes for the contributions of the different components are given in Fig. 3, with the yellow curve in panel **q**) showing the additional contribution by the halo component (C_{halo}) in front of the nuclear region of Arp 220.

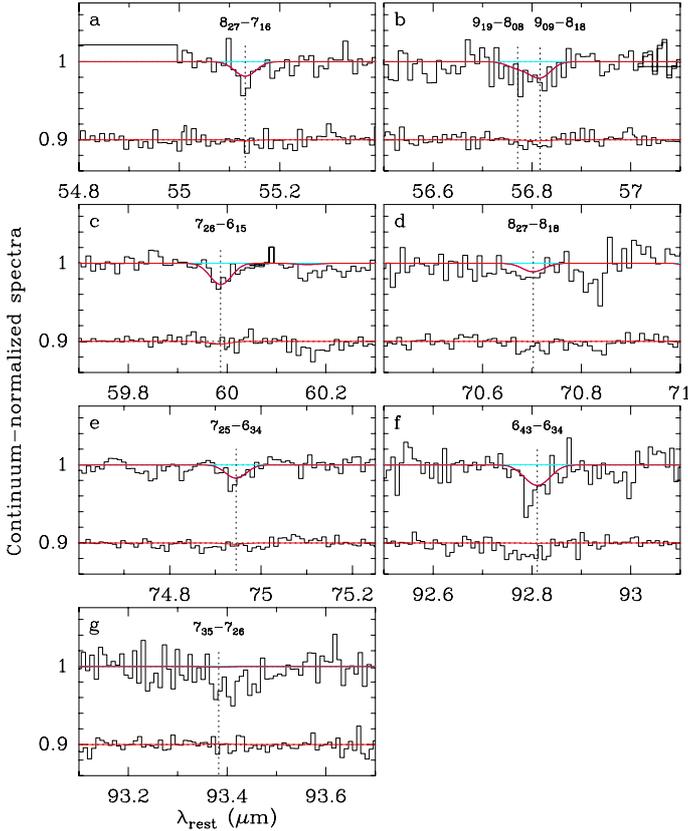


Fig. 5. Marginally detected H₂O lines in NGC 4418 (upper spectra in each panel); the corresponding lines from Arp 220 are also shown (lower spectra). Model predictions for these lines (for C_{core} in NGC 4418 and for C_{west} in Arp 220) are also shown (red curves).

and the $(3, K)s \rightarrow (2, K)a$ ($\approx 165.7 \mu\text{m}$, Fig. 10f) lines, up to $(10, K) \rightarrow (9, K)$ at $50\text{--}51 \mu\text{m}$.

Figure 10 also indicates (partial) blending with lines of other species, as H₂O (panels a and b), CH⁺ (panel b), and H₃O⁺ (panel f). Most $(6, K)a \rightarrow (5, K)s$ lines are strongly blended with the OH $84 \mu\text{m}$ doublet. From the comparison with the modeling described in Sect. 3, the $(6, K)s \rightarrow (5, K)a$ and especially the $(7, K)a \rightarrow (6, K)s$ lines are so blended that a pseudo-continuum is expected to be formed, with the consequent uncertainty in the baseline subtraction. As also found for H₂O, OH, and HCN, NGC 4418 shows in NH₃ clear indications of higher excitation than Arp 220, and the absorption in non-metastable levels relative to metastable ones is also stronger in NGC 4418 (e.g., the $(4, K)s \rightarrow (3, K)a$ group in panel d). The ortho-NH₃ $(8, 6)a \rightarrow (7, 6)s$ is probably detected in NGC 4418, as the blended para-H₂O $8_{08} \rightarrow 7_{17}$ line (see also Fig. 3f) is probably less strong than the close ortho-H₂O $8_{18} \rightarrow 7_{07}$ line, and also because the $(8, 6)s \rightarrow (7, 6)a$ transition is detected. There are also some hints of absorption in the $(8, 5)s \rightarrow (7, 5)a$ line. In summary, NH₃ lines are detected up to $(8, K) \rightarrow (7, K)$ in NGC 4418 ($E_{\text{lower}} \approx 600 \text{ K}$), and up to $(7, 6) \rightarrow (6, 6)$ in Arp 220 ($E_{\text{lower}} \approx 400 \text{ K}$).

2.7. Kinematics

In Fig. 12, we compare the HCO⁺ $J = 3\text{--}2$ (green histograms) and $J = 4\text{--}3$ (blue histograms) line profiles toward the western (a) and eastern (b) nucleus of Arp 220 (from Sakamoto et al. 2009), with the line profiles of selected lines detected with *Herschel*/PACS (c-i). The HCO⁺ lines toward both nuclei,

observed with high angular ($0.3''$) and spectral (30 km s^{-1}) resolution, exhibit P-Cygni profiles indicative of outflowing gas (Sakamoto et al. 2009). Specifically, the redshifted spectral features observed in emission have a large velocity extent of $\sim 500 \text{ km s}^{-1}$ from the systemic velocity. This prominent redshifted HCO⁺ emission has its counterpart in several lines detected with *Herschel*/PACS: the H₂O $3_{03} \rightarrow 2_{12}$ line at $174.6 \mu\text{m}$ (Fig. 12c), the [O I] $63 \mu\text{m}$ transition (d), and the OH $79 \mu\text{m}$ doublet (e). The latter also shows deeper absorption in the blue Λ -component than in the red one, suggesting the occurrence of redshifted emission in the blue Λ -component as well. The line emission features are expected to be formed in gas located at the back/lateral sides (i.e. not in front of the nuclei where absorption of the continuum dominates the profile), and will therefore be redshifted, as observed, if the gas is outflowing. The velocity of the emission features ($v_{\text{LSR}} \sim 5650\text{--}6000 \text{ km s}^{-1}$) is significantly higher than the redshifted velocities measured for the rotating disks around both nuclei (up to $\sim 5700 \text{ km s}^{-1}$, Sakamoto et al. 2008), indicating that little of this emission is associated with the rotation motions. Thus we conclude that moderate excitation lines of H₂O, OH, and O I trace the outflow at redshifted velocities detected in HCO⁺. The asymmetric shape of the OH $163 \mu\text{m}$ emission doublet, which peaks at redshifted velocities, is consistent with this scenario, as is the detection of redshifted emission features in the *Herschel*/SPIRE spectrum of Arp 220 in several species including H₂O (Rangwala et al. 2011).

The blueshifted velocity extent of the OH 163 and [O I] $145 \mu\text{m}$ lines, observed in emission, reaches $\sim 400 \text{ km s}^{-1}$ from the systemic velocity (Figs. 12h–i), and could also trace outflowing gas at the most extreme velocities. The full velocity extent in these lines ($\approx 1000 \text{ km s}^{-1}$) is similar to that of CO $(3\text{--}2)$ (Sakamoto et al. 2009). The full velocity extent of the high-lying H₂O lines is significantly lower, $\approx 550 \text{ km s}^{-1}$. This is specifically illustrated in Figs. 12f–g for the $3_{22} \rightarrow 2_{11}$ and $6_{16} \rightarrow 5_{05}$ lines, which lie in the range $90\text{--}82 \mu\text{m}$ where PACS has relatively high velocity resolution ($130\text{--}150 \text{ km s}^{-1}$). In contrast with the OH 163 and the [O I] $145 \mu\text{m}$ lines observed in emission, which probably trace spatially extended gas, the formation of the high-lying absorption H₂O lines is restricted to regions with high far-IR radiation densities that are optically thick at far-IR wavelengths, obscuring the emitting gas behind the nuclei. The absorption in these H₂O lines peaks at around central velocities, indicating that the lines mainly trace gas rotating on the surface of the nuclei. However, due to uncertainties in the velocity correction due to pointing shifts (see Sect. 2), and the similarity in the blueshifted velocity extent of the HCO⁺ and H₂O lines, we cannot rule out a significant contribution to the absorption by outflowing gas with velocities up to $\sim 150 \text{ km s}^{-1}$. Nor can we rule out spatially extended gas inflow, similar to what is inferred and discussed below for NGC 4418, since the peak absorption in the OH $79 \mu\text{m}$ doublet is redshifted by $\approx 90 \text{ km s}^{-1}$.

In NGC 4418, the adopted redshift ($z = 0.00705$) is derived from the excited H₂O and OH lines, coinciding within $\approx 15 \text{ km s}^{-1}$ with both the centroid of the [C II] $158 \mu\text{m}$ line and with the redshift inferred from the stellar absorption at optical wavelengths (Sect. 2.2). No indication of outflowing gas in the nuclear region is found. The excited H₂O and OH lines in NGC 4418 are indeed significantly narrower than in Arp 220 (Figs. 13 and 14), further indicating the relatively quiescent state of the NGC 4418 nucleus. On the other hand, the line shapes of the lowest-lying H₂O, OH, and [O I] lines show an intriguing behavior, opposite to the outflow signatures in Arp 220: the absorption features in the ground OH and [O I] $63 \mu\text{m}$ lines are

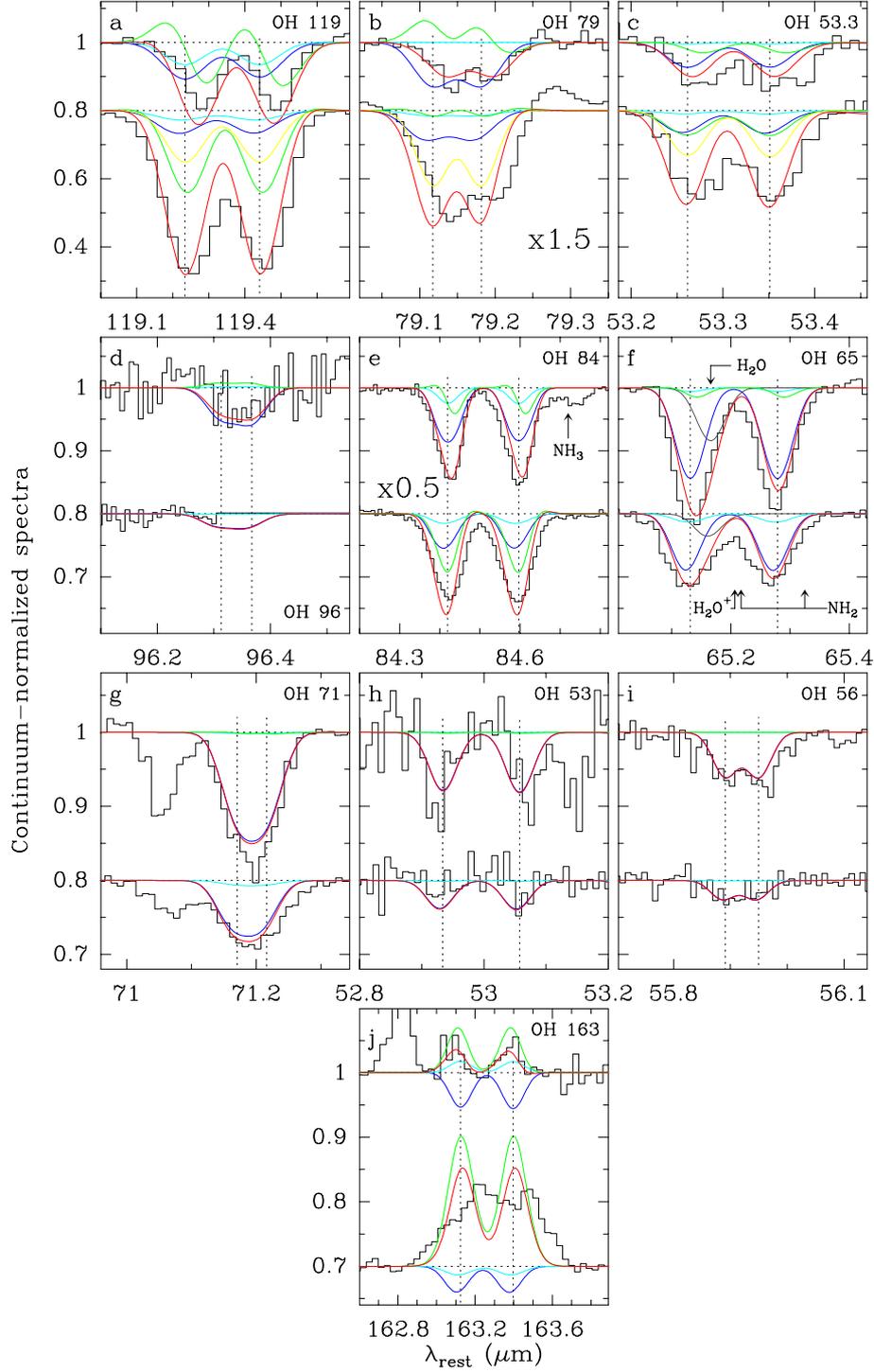


Fig. 6. OH lines in NGC 4418 (upper spectra) and Arp 220 (lower spectra). Λ -doubling is resolved in most transitions, except for the two narrowly separated $71 \mu\text{m}$ components that are blended into a single spectral feature. Model results are also shown. For NGC 4418, the blue, light-blue, and green curves show the models for the C_{core} , C_{warm} , and C_{extended} components, respectively; for Arp 220, the blue, light-blue, green, and yellow curves show the models for C_{west} , C_{east} , C_{extended} , and C_{halo} , respectively. The gray curves in panel f) show the expected contribution of the $\text{H}_2\text{O } 6_{25} \rightarrow 5_{14}$ line to the spectra around $65.2 \mu\text{m}$. The red curves show the total from all components.

systematically redshifted by $\sim 100 \text{ km s}^{-1}$, and the $[\text{O I}] 63 \mu\text{m}$ line shows a *blueshifted* spectral component in emission, peaking at $\approx -55 \text{ km s}^{-1}$, i.e. an inverse P-Cygni profile (Fig. 11a). The lowest-lying H_2O line at $179.5 \mu\text{m}$ is also redshifted, but contamination by $\text{CH}^+ (2 \rightarrow 1)$ at $179.594 \mu\text{m}$ makes the case more uncertain. Additional clues about this component come from the line shapes of the OH 84 and $163 \mu\text{m}$ doublets: the

blue Λ -component of the $84 \mu\text{m}$ doublet ($E_{\text{lower}} = 121 \text{ K}$) shows an asymmetric shape with some redshifted excess (Figs. 6e and 11e; the red Λ -component is probably contaminated by excited NH_3 , see Fig. 10c), suggesting that some redshifted gas at $\sim 50 \text{ km s}^{-1}$ is significantly excited. The kinematics implied by the OH $163 \mu\text{m}$ emission doublet are unclear due to the low signal-to-noise ratio (SNR), as one of the components is

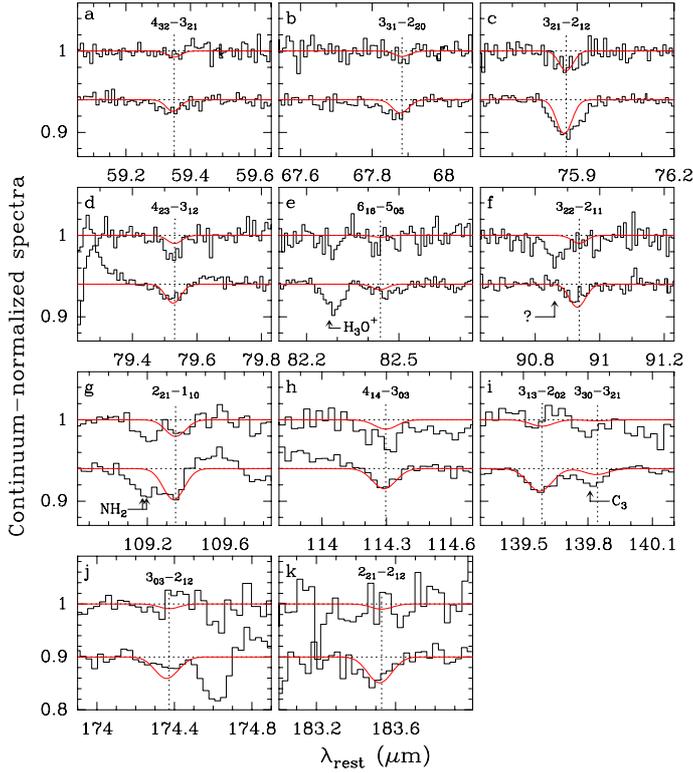


Fig. 7. Spectra around the wavelengths of relevant H₂O lines in NGC 4418 (upper profiles) and Arp 220 (lower profiles). Model predictions for NGC 4418 (C_{core}) with $\text{H}_2\text{O}/\text{H}_2^{18}\text{O} = 500$, and for Arp 220 (C_{west}) with $\text{H}_2\text{O}/\text{H}_2^{18}\text{O} = 70$ are shown in red.

apparently *blueshifted*, whereas the other one peaks at central velocities (Figs. 6j, 11f, and 14). In summary, the ground-state lines of OH and [O I], together with the OH 84 and 163 μm doublets, indicate the presence of a component different from the nuclear one in both excitation and kinematics, most probably extended in comparison with the nucleus but much less massive than the C_{extended} component of Arp 220, and the velocity shifts suggest that this component may be *inflowing* onto the quiescent, nuclear region. We further investigate this scenario in Sect. 3.6.

3. Models

3.1. Overview

As the data presented in previous sections have shown, the far-IR spectra of NGC 4418 and Arp 220 are dominated by molecular absorption, with emission in only some lines and profiles. These rich line spectra and their associated dust emission cannot be described by a single set of ISM parameters, but different lines have different excitation requirements and are thus formed in different regions of the galaxies. Our approach for both galaxies is to fit these different regions and conditions, even though they are not spatially resolved with *Herschel*, with the smallest possible number of parameterized components.

For NGC 4418, we find that we need (see Fig. 1a) (i) a hot component (yellow curve, hereafter C_{hot}) that accounts for the mid-IR continuum; (ii) a nuclear core (blue curve, C_{core}) that provides absorption in the high-lying lines of H₂O, OH, HCN, and NH₃; (iii) a warm component (light-blue, C_{warm}), that provides absorption in moderately excited lines of H₂O and OH as well as a significant fraction of the far-IR continuum emission;

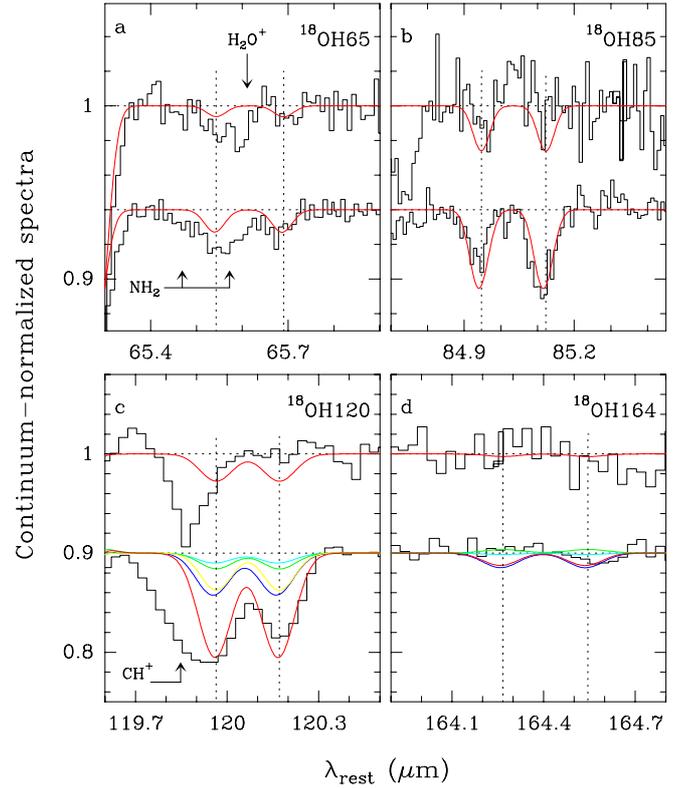


Fig. 8. Spectra around the wavelengths of relevant ¹⁸OH lines in NGC 4418 (upper profiles) and Arp 220 (lower profiles). Model predictions for NGC 4418 (C_{core}) with $\text{H}_2\text{O}/\text{H}_2^{18}\text{O} = 500$, and for Arp 220 with $\text{H}_2\text{O}/\text{H}_2^{18}\text{O} = 70$ are also shown. For the ¹⁸OH 120 μm doublet, the contributions by the different components in Arp 220 (see Fig. 6) are indicated; red denotes the total of all components.

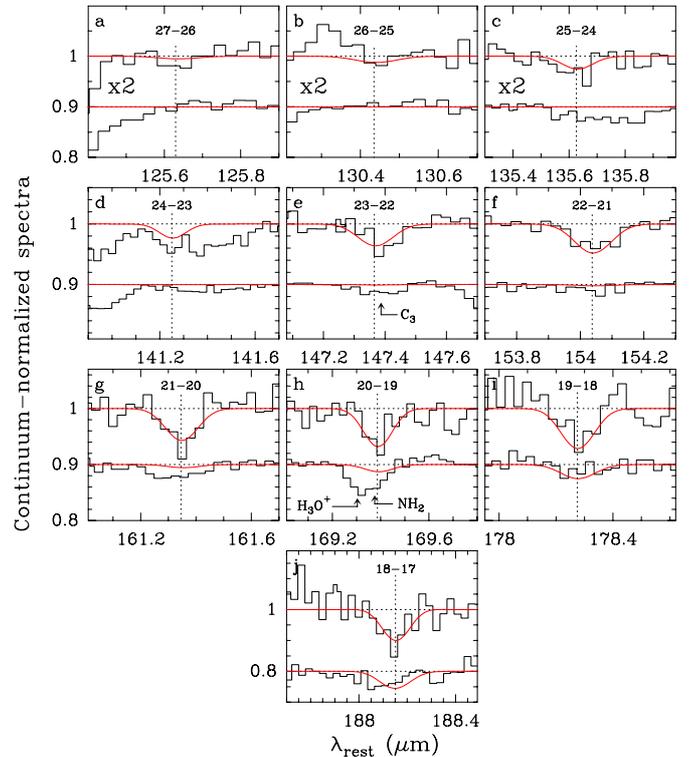


Fig. 9. Spectra around the frequencies of HCN lines in NGC 4418 (upper profiles in each panel) and Arp 220 (lower profiles). Model predictions for NGC 4418 (C_{core}) and Arp 220 (C_{west}) are included.

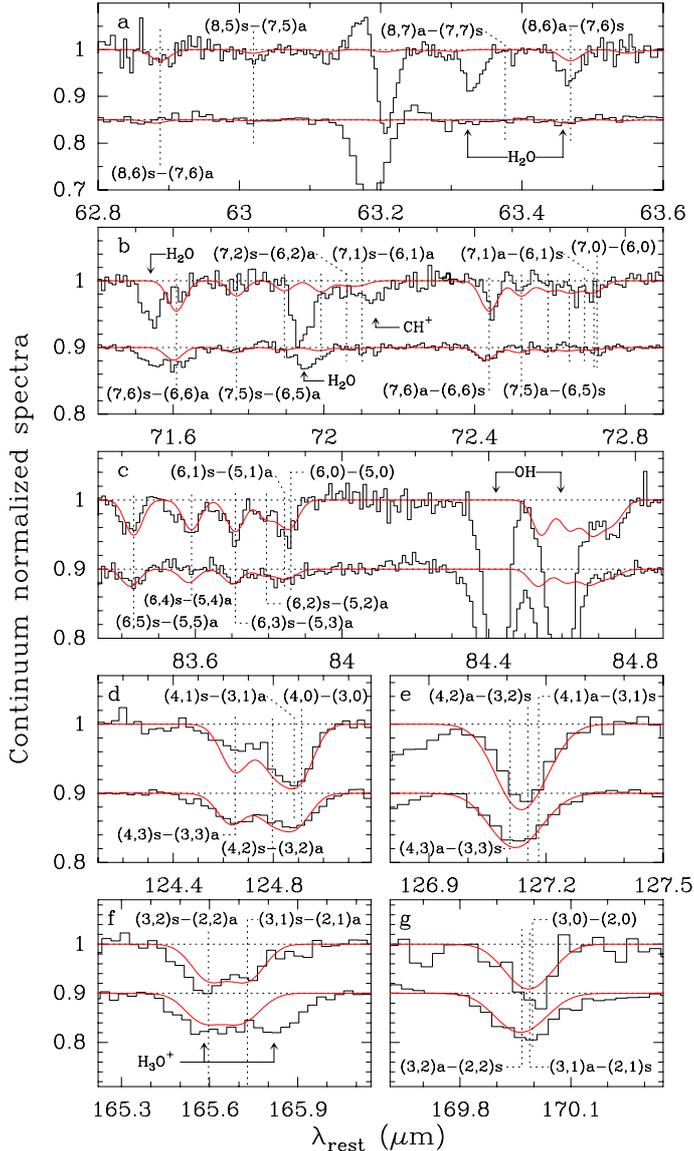


Fig. 10. Spectra around the frequencies of relevant NH_3 lines in NGC 4418 (upper profiles in each panel) and Arp 220 (lower profiles). Model predictions for NGC 4418 (C_{core}) and Arp 220 (C_{west}) are included.

and (iv) an extended component (solid green, C_{extended}), which accounts for the low-lying redshifted lines of OH and O I.

For Arp 220, we need (Fig. 1b) (i) a single³ hot component (yellow curve, C_{hot}) that accounts for the mid-IR continuum emission; (ii) the western and eastern nuclear components (C_{west} and C_{east} in blue and light blue, respectively), where the high-lying molecular lines are formed; (iii) the extended component (C_{extended} , green), which provides a significant fraction of the far-IR continuum emission and which is likely associated with moderate and low-excitation lines of H_2O and OH; and (iv) an additional absorbing “halo” component (C_{halo}), with no associated intrinsic continuum but located in front of the nuclei, is required to fit the absorption in the ground-state lines of H_2O , OH, and O I.

³ Even if the mid-IR arises from the two nuclei, the continuum is simulated with just a single component with an effective diameter as given in Table 1.

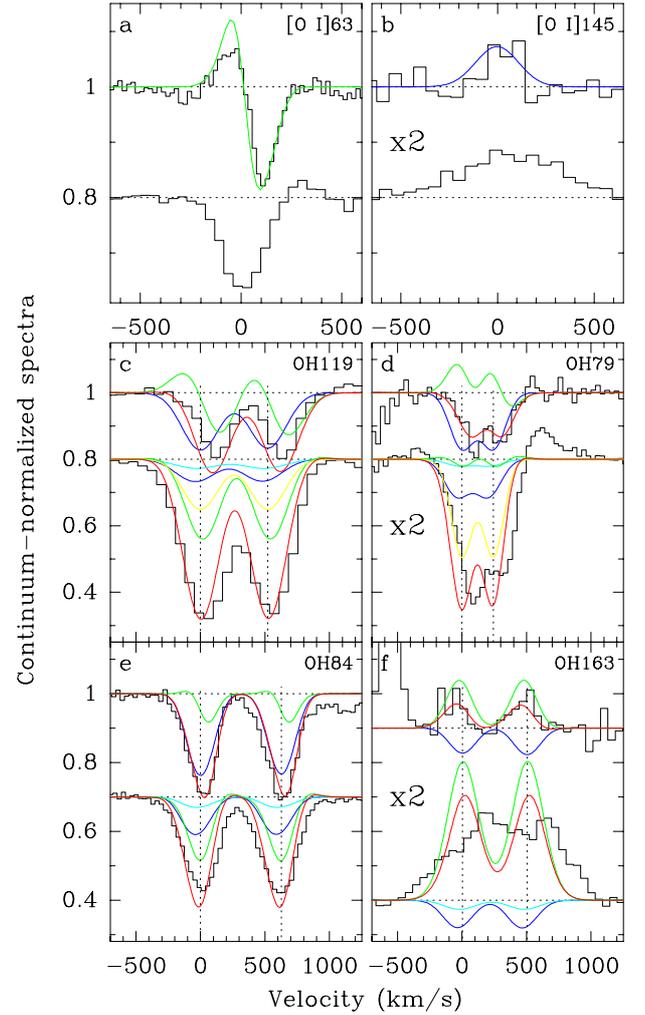


Fig. 11. Line profiles of the [O I] 63 and 145 μm (a and b) transitions compared with those of some OH lines (c–f). Upper histograms, NGC 4418; lower histograms, Arp 220. Model predictions are also included. For NGC 4418, the blue curves show the combined contribution of the C_{core} and C_{warm} components, and the green curves show the model for C_{extended} . For Arp 220, see caption of Fig. 6. Red denotes the total of all components.

We use single dust temperatures for every component listed above, except for the C_{extended} component in both galaxies where the dust temperature profile is calculated from the balance of heating (by the inner components) and cooling (González-Alfonso & Cernicharo 1999). In our models, each single dust temperature component is attenuated by a foreground, screen-like shell, which is parameterized by its dust opacity at 25 μm , $\tau_{25,\text{fg}}$. These screen-like shells are responsible for the silicate absorption features imprinted on the various modeled components in Fig. 1. The dust temperature profile in C_{extended} is calculated by assuming spherical symmetry and a single nuclear heating component located at the center of the modeled source.

Parameters of the continuum models, and the inferred molecular parameters, are listed in Tables 1 and 2, respectively. A sketch of the modeled sources, showing the approximate spatial scales of the different far-IR components (excluding the C_{hot} component of both galaxies), is shown in Fig. 16. Each component, however, can be interpreted in terms of a single source, as implicitly assumed, or alternatively applied to each one of an ensemble of N_C smaller clouds of radius R_C that do not spatially

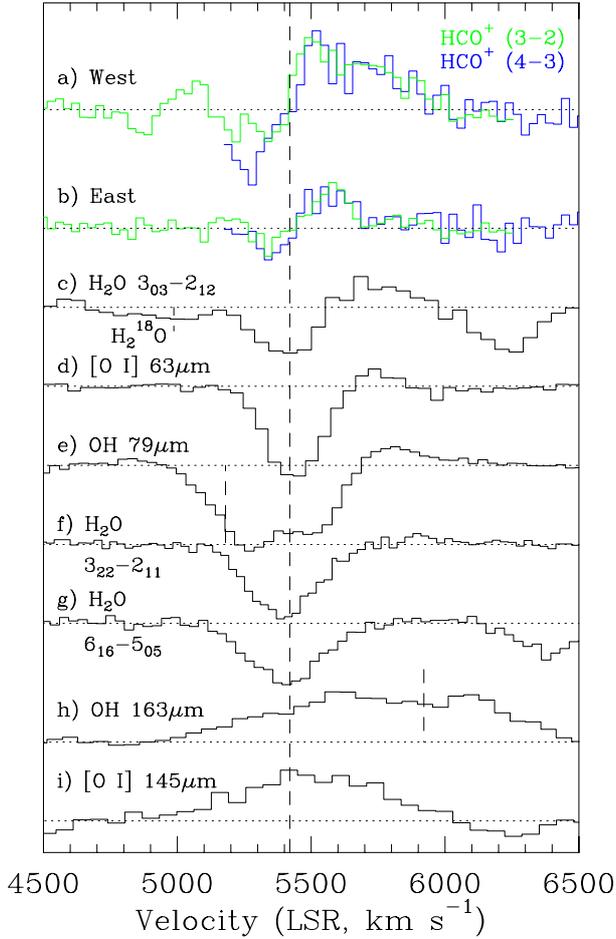


Fig. 12. Comparison between the line shapes of the HCO^+ $J = 3 \rightarrow 2$ (green histograms) and $J = 4 \rightarrow 3$ (blue histograms) transitions toward **a)** the western and **b)** eastern nucleus of Arp 220 (from Sakamoto et al. 2009), with selected lines detected with *Herschel*/PACS (**c**–**i**). The dashed vertical line indicates our adopted systemic velocity (Sect. 2.2). The velocity scale for the OH 79 (163 μm) doublet is relative to the red (blue) Λ -component, and the systemic velocity for the other Λ -component is also indicated. The velocity of the H_2^{18}O $3_{03} \rightarrow 2_{12}$ line in **c)** is also indicated.

overlap along the line of sight. The scaling between these two approaches is discussed in G-A04.

The models for Arp 220 are discussed in Sects. 3.2 (high-lying lines) and 3.3 (low-lying lines), while those for NGC 4418 are developed in Sects. 3.4 (high-lying lines), 3.5 (mid-excitation lines), and 3.6 (low-lying lines). The continuum of NGC 4418 is further discussed in 3.7.

3.2. The high-lying lines in Arp 220: the nuclear region (C_{west} and C_{east})

3.2.1. H_2O

Our models for Arp 220 are similar to those described in G-A04, and generated on the basis of the interplay between the continuum emission and the molecular line absorption. Since the molecular excitation in Arp 220 is high and collisional excitation alone cannot account for it, the excitation mechanism is expected to be dominated by absorption of dust-emitted photons in the nuclear region of the galaxy (G-A04, González-Alfonso et al. 2008, 2010). The molecular excitation is thus a function of the

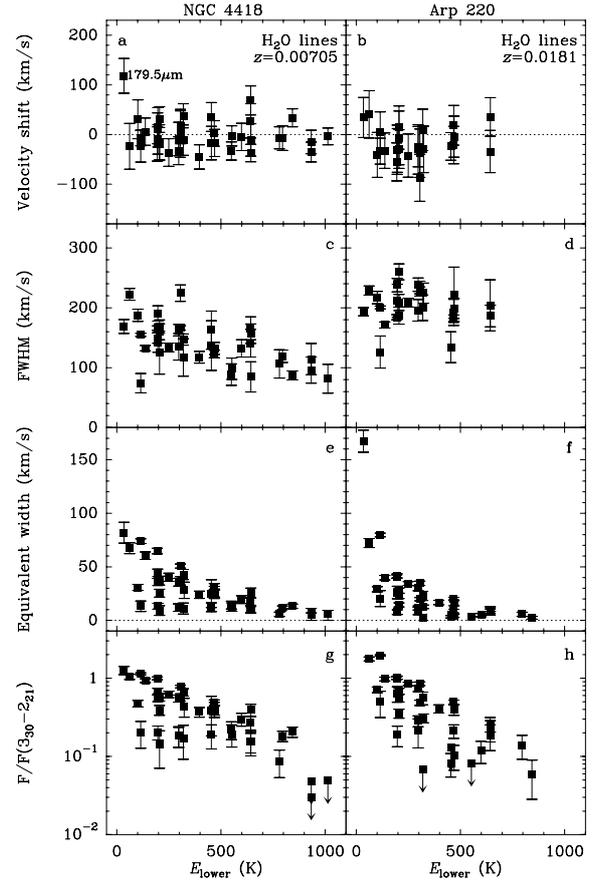


Fig. 13. Velocity shifts (**a**–**b**), line widths (**c**–**d**), and equivalent widths (**e**–**f**) of the H_2O lines in NGC 4418 (*left*) and Arp 220 (*right*). Panels **g**–**h** show the line fluxes normalized to that of the $3_{30} \rightarrow 2_{21}$ transition at 66.4 μm (see Sect. 2.3 for details). Error bars are $1\text{-}\sigma$ uncertainties from Gaussian fits to the lines.

dust temperature, T_{d} , and of $N_{\text{H}_2\text{O}}/\Delta v$, and in combination with the observed continuum provides clues about the general properties of the far-IR continuum source and its associated chemistry. If the observed H_2O excitation cannot be reproduced by assuming that the dust in the nuclear component has a temperature of “only” $T_{\text{d}} = 85$ K (derived from the *observed* 25 and 1300 μm emission), foreground extinction in the far-IR is included to attenuate also the 25 μm emission from the nuclei in such a way that the far-IR is reproduced with $T_{\text{d}} > 85$ K. This is Scenario 2, S_2 , in G-A04, based on the continuum models by Soifer et al. (1999). Evidence for such foreground extinction in the mid-IR comes from the strong silicate absorption at 9.7 and 18 μm , in the millimeter by self-absorption in CO ($2 \rightarrow 1$) (Downes & Eckart 2007), and in the far-IR from the [O I] 63 μm line that is observed in absorption, in contrast to most extragalactic sources in which it is observed in emission.

In the present models, we have simulated the dust emission by using a mixture of silicate and amorphous carbon grains with optical constants from Draine (1985) and Preibisch et al. (1993); the mass-absorption coefficient is 550, 150, and 12.3 cm^2/g of dust at 25, 50, and 200 μm , respectively, and the spectral index is $\beta \approx 2$ in the far-IR. We have also attempted to disentangle the emission from the eastern and western nuclei in Arp 220. We have modeled the eastern nucleus (C_{east}) as a sphere of diameter $d_{\text{east}} = 0.31''$ (Sakamoto et al. 2008, hereafter Sa08), radial opacity (i.e. the opacity along a radial path) at 200 μm $\tau_{200} = 2.7$, and $T_{\text{d, east}} = 87$ K. The emission from

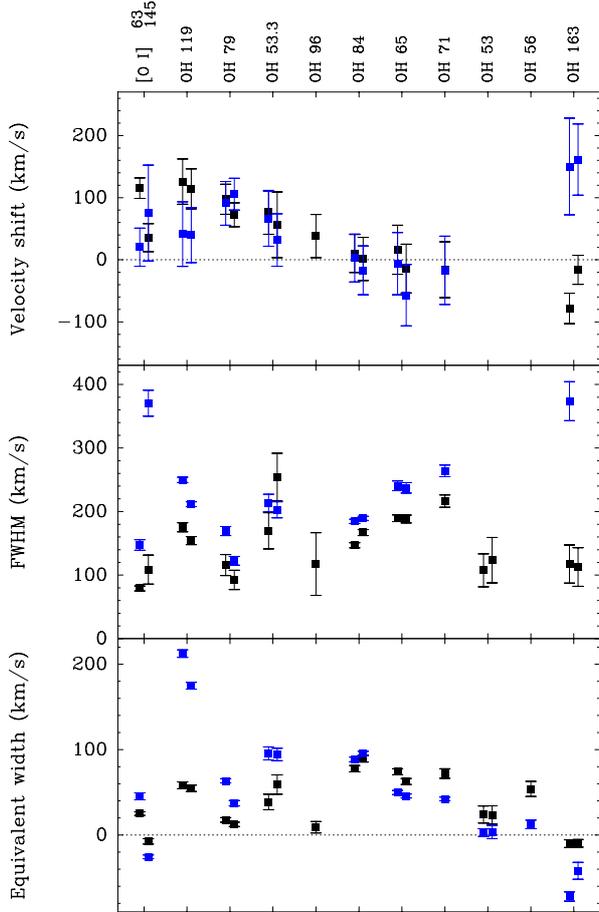


Fig. 14. Velocity shifts, line widths, and equivalent widths of the [O I] and OH lines in NGC 4418 (black symbols) and Arp 220 (blue symbols). Error bars are $1\text{-}\sigma$ uncertainties from Gaussian fits to the lines.

C_{east} is attenuated by foreground dust with $\tau_{25,\text{fgr}} = 1$, yielding $2.5\text{--}0.02$ Jy at $25\text{--}1300$ μm – consistent with measurements by Soifer et al. (1999) and Downes & Eckart (2007). The corresponding SED of C_{east} is shown in Fig. 1b in light-blue, and accounts for a luminosity of $L_{\text{east}} = 3 \times 10^{11} L_{\odot}$. For the western nucleus (C_{west}) we also use as a first approach the size as derived by Sa08 in the “disk” approximation, i.e. a sphere with diameter $d_{\text{west}} = 80$ pc ($0.23''$ at 72 Mpc), but allow it to vary to match the observed continuum, and leave as free parameters the dust temperature $T_{\text{d,west}}$ and foreground extinction $\tau_{25,\text{fgr}}$.

Calculations for the lines were carried out in spherical symmetry using the code described in González-Alfonso & Cernicharo (1999). The models indicate that most high-lying absorption lines are formed in the outermost shell surrounding the far-IR continuum source. This is illustrated in Fig. 17, where the absorbing flux of several lines of H_2O , OH, H_2^{18}O , NH_3 , and HCN, is plotted as a function of the depth of the shell where the molecules are located, which is parameterized in terms of the continuum opacity at 50 μm (τ_{50}) measured from the surface of the far-IR source. Since the molecular abundances relative to the density of dust are uniform in these models, the column densities are proportional to τ_{50} . Results indicate that the H_2O and OH absorption is produced in a thin shell with $\tau_{50} \approx 1$, as extinction, thermalization by dust emission, as well as line opacity effects make results insensitive to the presence of molecules deeper into the far-IR source. The optically thinner H_2^{18}O lines are mostly formed in the same shell, though the lines at long wavelengths

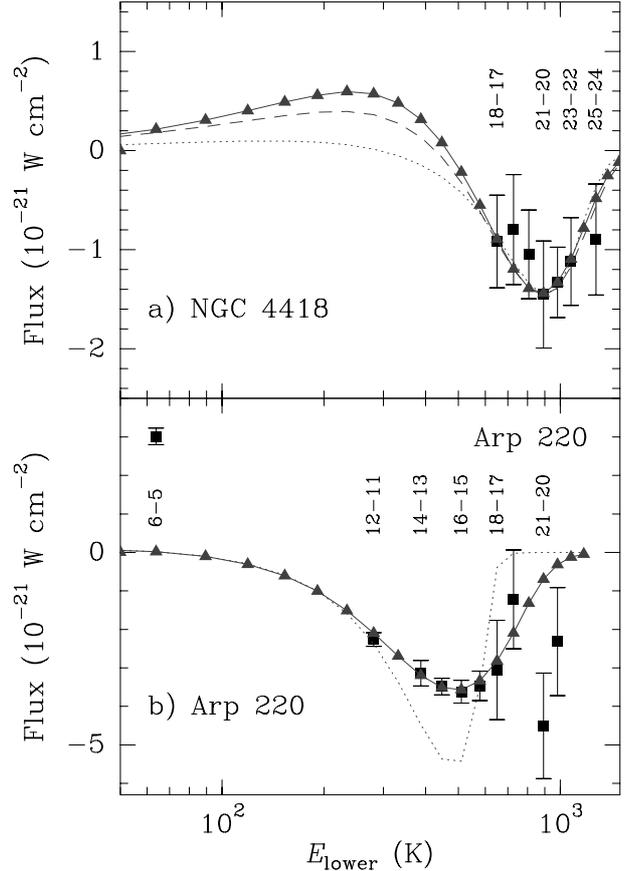


Fig. 15. HCN line fluxes in NGC 4418 **a)** and Arp 220 **b)**. In Arp 220, the fluxes of lines with E_{lower} up to 570 K have been taken from SPIRE-FTS data (Rangwala et al. 2011). The curves and triangles show model predictions for the C_{core} component of NGC 4418 and the C_{west} component of Arp 220. The dotted curve in **b)** shows results obtained when only collisional excitation is included in the model. The solid curve in **a)** shows the best fit model obtained with $\tau_{200} \approx 1$, while the dashed and dotted curves correspond to $\tau_{200} = 4$ with and without gas-dust mixing, respectively.

(e.g. the $2_{21} \rightarrow 2_{12}$ at 183 μm) still have significant contribution ($\lesssim 25\%$) from the $1 < \tau_{50} < 2$ region. The case for NH_3 and HCN is somewhat different, as some lines probe deeper regions. The high-lying lines of NH_3 lie at $\lambda < 100$ μm and are also formed in the $\tau_{50} \approx 1$ outermost shell, but the low-lying lines at $\lambda > 100$ μm have significant contribution from $1 < \tau_{50} < 3$. The high-excitation HCN lines sample regions deeper than the other species ($\tau_{50} \lesssim 4$) as their excitation is sensitive to the far-IR radiation density at $\lambda \gtrsim 170$ μm (see Sect. 3.2.4). Based on these results, the models for the nuclei shown below use a “screen” approach, i.e. the molecules are mixed with the dust but located within a thin shell surrounding the nuclei extended up to a depth of $\tau_{50} = 2$ for H_2O , OH, and their ^{18}O isotopologues, and up to $\tau_{50} = 4$ for NH_3 and HCN. The values of the column densities of all species below, however, are given for the $\tau_{50} = 1$ outermost shell that dominates the absorption of H_2O and OH, and are lower limits to the true columns through the nuclear sources. In order to estimate the abundances χ_X relative to H nuclei, we have normalized these column densities per unit of τ_{50} to a given value of $N_{\text{H, norm}}$. For a mass-absorption coefficient of 150 cm^2/g of dust at 50 μm and a gas-to-dust mass ratio of 100, $\tau_{50} = 1$ corresponds to a column density of $N_{\text{H, norm}} = 4 \times 10^{23}$ cm^{-2} , where H refers to hydrogen nuclei in both atomic and molecular

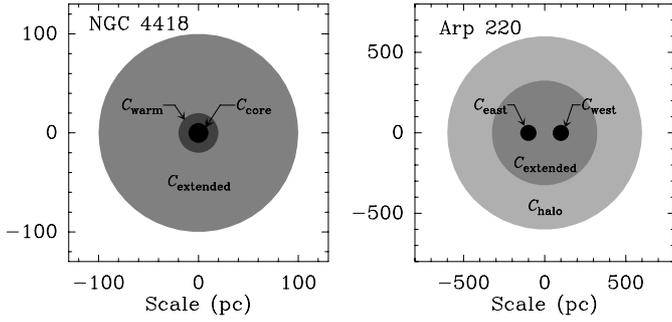


Fig. 16. Schematic representation of the modeled spatial scales of the different far-IR sources (see Fig. 1 and Tables 1 and 2). The C_{hot} components in both galaxies (that account for the mid-IR spectra) are most probably associated with the nuclear regions and are not included here. The C_{halo} component in Arp 220 has no associated continuum, and is responsible for the absorption of the nuclear continuum (C_{east} and C_{west}) in the ground-state lines of H_2O , OH, and O I. Although, due to its apparent low excitation, C_{halo} is represented here as the most extended component, its size is not constrained. The plot is an oversimplification of the actual models, where the different components are modeled separately to account approximately for non-spherical symmetry.

forms. This value of $N_{\text{H},\text{norm}}$ has been applied to all species observed in the far-IR, and define the far-IR “photosphere” where most molecular absorption is produced.

Line broadening is caused by microturbulence with $v_{\text{turb}} = 60 \text{ km s}^{-1}$ and a velocity shift of 130 km s^{-1} through the absorbing shell. The latter simulates either the presence of outflowing gas or, more generally, gas velocity gradients across the nuclear regions, allowing us to nearly match the observed linewidths. Rates for collisional excitation are taken from Faure et al. (2007); with the adopted $n_{\text{H}_2} = 5 \times 10^5 \text{ cm}^{-3}$ and gas temperature $T_{\text{g}} = 150 \text{ K}$ (see Sect. 3.2.4), collisional excitation has little effect on the calculated fluxes. The line models have three free parameters: the dust temperature, T_{d} , the H_2O column, $N_{\text{H}_2\text{O}}$, and the covering factor of the continuum source, f_{c} .

The bulk of the H_2O absorption is produced in a luminous, compact region with high H_2O columns, which we identify with the double nucleus of Arp 220. A number of previous observational studies with high angular resolution have revealed that the western nucleus is brighter than the eastern one in the near-IR (Armus et al. 1995), mid-IR (by a factor of ~ 3 at $25 \mu\text{m}$; Soifer et al. 1999), and (sub)millimeter wavelengths (Downes & Eckart 2007; Sakamoto et al. 2008). Given that the excitation of H_2O requires a high brightness continuum source, the observed high-lying H_2O absorption is tentatively attributed to C_{west} . Nevertheless, the column densities derived below are independent of whether C_{west} alone is responsible for the absorption in the high-lying lines, or C_{east} has a significant contribution as well, and the properties we derive for C_{west} and C_{east} can be more generally interpreted as shared by both nuclei.

In the nuclear region where the H_2O lines are formed, the models shown below indicate that most of these lines are strongly saturated; however, there are still some high-lying lines that are sensitive to both $N_{\text{H}_2\text{O}}$ and T_{d} . For these critical lines, Fig. 18 shows the observed and modeled fluxes relative to that in the $3_{30} \rightarrow 2_{21}$ line at $66.4 \mu\text{m}$ (Fig. 3g). As mentioned in Sect. 2, the $3_{30} \rightarrow 2_{21}$ is chosen as the normalization line because it is detected with a high SNR and, with $E_{\text{lower}} = 160 \text{ K}$, is not expected to be significantly contaminated by absorption of extended low-excitation H_2O in Arp 220. On the other hand, the $3_{30} \rightarrow 2_{21}$ transition is still low in energy as compared with the high-lying lines,

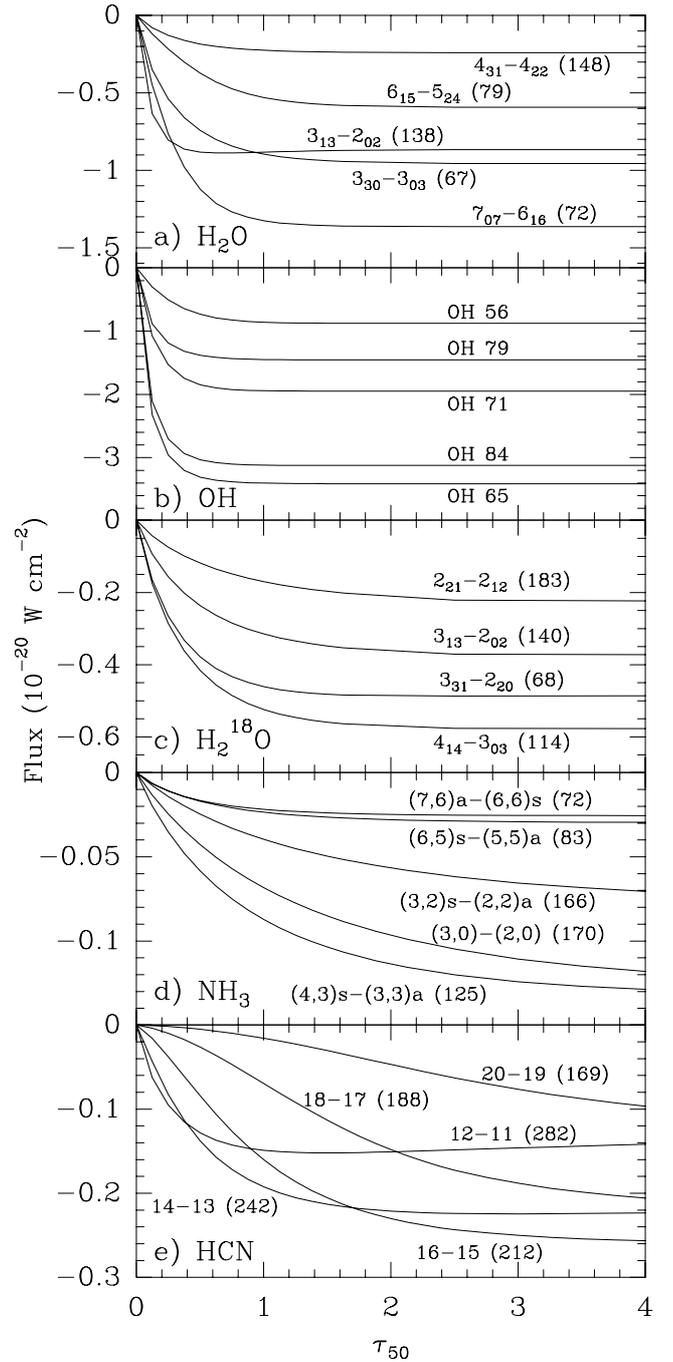


Fig. 17. Modeled absorbing flux in Arp 220 of several a) H_2O , b) OH, c) H_2^{18}O , d) NH_3 , and e) HCN lines as a function of the depth of the molecular shell measured from the surface of the continuum source, as parameterized by the dust opacity at $50 \mu\text{m}$ (τ_{50}). Numbers in parenthesis indicate rounded wavelengths in μm . The total column of molecules is proportional to τ_{50} , and we have adopted $N_{\text{H}_2\text{O}} = 2 \times 10^{18} \times \tau_{50} \text{ cm}^{-2}$, and abundance ratios of $\text{OH}/\text{H}_2\text{O} = 0.5$, $\text{H}_2\text{O}/\text{H}_2^{18}\text{O} = 100$, $\text{HCN}/\text{H}_2\text{O} = 0.3$, and $\text{HCN}/\text{NH}_3 = 6$. The dust temperature is 110 K .

so that the line flux ratios are sensitive to both $N_{\text{H}_2\text{O}}$ and T_{d} . Furthermore, the line flux ratios do not depend on either the size of the continuum source, or on f_{c} . These ratios are plotted as a function of T_{d} for different “screen-like” H_2O columns, ranging from $N_{\text{H}_2\text{O}} = 7.5 \times 10^{17}$ to $6 \times 10^{18} \text{ cm}^{-2}$, with dashed lines indicating the measured values, and dotted lines the estimated upper and lower limits. We also include in the lowest panel the upper limit derived for the $8_{18} \rightarrow 7_{07}$ line. For each T_{d} , the foreground

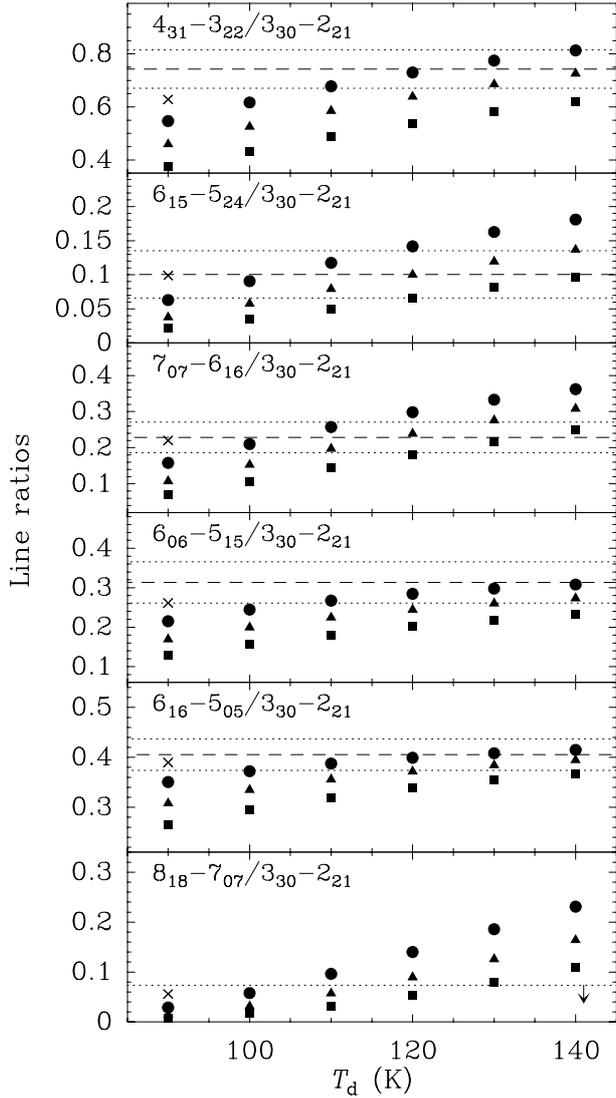


Fig. 18. Modeled H₂O line ratios in Arp 220 as a function of the dust temperature in the western nucleus. The dashed lines indicate the observed values, and the dotted lines the estimated upper and lower limits. In the lowest panel, the dotted line is the 3σ upper limit for the $8_{18}-7_{07}/3_{30}-2_{21}$ flux ratio. Squares, triangles, circles, and crosses (only for $T_{d,\text{west}} = 90$ K) show model results for “screen” H₂O columns of $N_{\text{H}_2\text{O}} = 7.5 \times 10^{17}$, 1.5×10^{18} , 3×10^{18} , and 6×10^{18} cm⁻², respectively.

extinction is determined by imposing that the continuum flux density at $25 \mu\text{m}$ matches the observed 7.5 Jy from the western nucleus (Soifer et al. 1999), but this has little effect on the line flux ratios as the far-IR foreground opacities are low and, in any case, the considered lines have similar wavelengths. The minimum T_d is 90 K, which is the optically thick, lower limit value derived for the western nucleus from the $860 \mu\text{m}$ submillimeter continuum by Sa08.

Results of Fig. 18 show that the line ratios scale linearly with T_d . The highest sensitivity to T_d is found for the $6_{15} \rightarrow 5_{24}$ line, since its lower level is non-backbone (Fig. 2). Among the detected lines, the line ratios can be almost equally well reproduced with $T_d = 90$ K and the highest $N_{\text{H}_2\text{O}} = 6 \times 10^{18}$ cm⁻², or with $T_d = 140$ K and $N_{\text{H}_2\text{O}} = 7.5 \times 10^{17}$ cm⁻². However, the model $T_d = 140$ K and $N_{\text{H}_2\text{O}} = 7.5 \times 10^{17}$ cm⁻² yields too much absorption in the undetected $8_{18} \rightarrow 7_{07}$ line, slightly favoring $T_d \lesssim 130$ K. Concerning the continuum models, if we

assume that the observed high-lying H₂O absorption is dominated by C_{west} , and that the photosphere at $25 \mu\text{m}$ has the same size as the (sub)millimeter source, a reasonable match to the $20\text{--}35 \mu\text{m}$ SED with $T_{d,\text{west}} \leq 110$ K is not possible; for example, the model with $T_{d,\text{west}} = 90$ K yields ≈ 4 Jy at $25 \mu\text{m}$ with no foreground extinction and the size derived from the submillimeter (Sa08), insufficient to account for the observed 7.5 Jy at $25 \mu\text{m}$ (Soifer et al. 1999). Furthermore, any reasonable fit to the continuum requires foreground absorption at $20\text{--}35 \mu\text{m}$, and the absolute H₂O fluxes also require a continuum source larger than the submillimeter one for $T_{d,\text{west}} \lesssim 120$ K. However, the photosphere at $25 \mu\text{m}$ (i.e. the nuclear region with $\tau_{25} \geq 1$) may be larger and colder than the submillimeter source if heated by the central core (Sa08), because the optically thinner submillimeter emission samples warm regions that are obscured at $25 \mu\text{m}$. For $T_{d,\text{west}} = 90$ K, the required source diameter is $d_{\text{west}} = 150$ pc, yielding $L_{\text{west}} = 6.5 \times 10^{11} L_{\odot}$, while for $T_{d,\text{west}} = 130$ K, $d_{\text{west}} = 80$ pc and $L_{\text{west}} = 8.2 \times 10^{11} L_{\odot}$.

In summary, a range of $T_{d,\text{west}} = 90\text{--}130$ K and a corresponding “screen” column per unit of τ_{50} of $N_{\text{H}_2\text{O}} = (60\text{--}7.5) \times 10^{17}$ cm⁻² are derived, with the colder (<120 K) sources yielding diameters above the (sub)millimeter observed values. The corresponding luminosities are in the relatively narrow range $L_{\text{west}} = (6.5\text{--}8.2) \times 10^{11} L_{\odot}$. The corresponding estimated H₂O abundances are $\chi_{\text{H}_2\text{O}} \sim (15\text{--}2) \times 10^{-6}$ relative to H nuclei.

As the reference model shown in Figs. 3–5 for detailed comparison with data, we use the combination $T_{d,\text{west}} = 110$ K and $N_{\text{H}_2\text{O}} = 2 \times 10^{18}$ cm⁻², with nearly complete coverage of the source ($f_C = 0.8$). The corresponding continuum is shown with a blue curve in Fig. 1b, with the diameter of the source (106 pc) increased by $\sim 30\%$ relative to the submillimeter source, and with a foreground opacity $\tau_{25,\text{fgf}} = 1.4$. The data also suggests the presence of a lower excitation component to attain a better fit to the $3_{22} \rightarrow 2_{11}$, $2_{21} \rightarrow 1_{10}$, and $3_{03} \rightarrow 2_{12}$ lines at 90, 108, and $174 \mu\text{m}$, respectively. Tentatively associating this component with the eastern nucleus, we derive $N_{\text{H}_2\text{O}} = 3 \times 10^{17}$ cm⁻² and $f_C = 0.4$. Its contribution to the H₂O SLED, shown with light-blue curves in Figs. 3 and 4, is expected to be significant only for low-lying H₂O lines. Continuum and line parameters of the models are listed in Tables 1 and 2.

3.2.2. OH

The observed high-lying OH doublets in Arp 220, namely the $\Pi_{3/2} 9/2 \rightarrow 7/2$ and $11/2 \rightarrow 9/2$ at 65 and $53 \mu\text{m}$, and the $\Pi_{1/2} 7/2 \rightarrow 5/2$ and $9/2 \rightarrow 7/2$ at 71 and $56 \mu\text{m}$, are compared in Fig. 6 (lower spectra) with the models for the western and eastern nuclei (blue and light-blue curves). Collisional rates between OH and H₂ were taken from Offer et al. (1994). As for H₂O, the absorption in these lines is dominated by a source with high OH column, which we tentatively identify with C_{west} . In the model of Fig. 6, we have used the same parameters as for H₂O, and varied the OH column density to match the observed absorption in the high-lying lines. We derive a OH/H₂O abundance ratio of 0.5–1; higher OH columns overpredict the absorption in the OH $53 \mu\text{m}$ doublet (Fig. 6h). The fit to the high-lying OH lines is satisfactory except for the underprediction of the width of the $\Pi_{3/2} 9/2 \rightarrow 7/2$ $65 \mu\text{m}$ doublet, which is probably contaminated by relatively weak lines of H₂O (gray curve in Fig. 6f), NH₂, and H₂O⁺. Using the same source sizes as for H₂O, we find a similar OH/H₂O $\sim 0.5\text{--}1$ ratio for $T_d = 90\text{--}130$ K. An additional extended region is required to fit the low-lying OH lines, which is discussed in Sect. 3.3.

3.2.3. H₂¹⁸O and ¹⁸OH

Although the detected H₂¹⁸O lines arise from low-lying levels, we find that these absorption features are mainly produced toward the nuclear region with the highest column densities. Figure 7 shows the best fit for the H₂¹⁸O lines using the same reference model as for the main isotopologue, i.e. $T_d = 110$ K. The best fit H₂¹⁸O column density is $\approx 3 \times 10^{16}$ cm⁻², implying an H₂¹⁶O-to-H₂¹⁸O ratio as low as ~ 70 , and the upper limit for this ratio is estimated to be ≈ 95 . The H₂¹⁶O-to-H₂¹⁸O ratio slightly depends on the dust temperature, and a value of ≈ 100 – 150 is found for the model with $T_d = 90$ K, though the overall fit is in this case less satisfactory. Thus our data suggest an enhancement of ¹⁸O in Arp 220 relative to the solar value of ~ 5 . This is confirmed by the models for ¹⁸OH shown in Fig. 8, where the same ¹⁶OH-to-¹⁸OH ratio of 70 is used with $T_d = 110$ K. The ¹⁶OH-to-¹⁸OH ratio would also increase up to 120–150 K for $T_d = 90$ K. The ¹⁸OH 65 and 85 μ m lines are nearly reproduced, but not the asymmetry in the ¹⁸OH 85 μ m doublet (Fig. 8b). Similar intensity asymmetries of $\approx 40\%$ have been also observed in most OH Λ -doublets by Goicoechea et al. (2011) toward the Orion bar, where the lines are observed in emission. As Goicoechea et al. (2011) indicate, this is probably due to asymmetries in the collisional rates between OH and para-H₂ (see also Offer et al. 1994). In our absorption lines, the asymmetry would arise from the collisional excitation of ¹⁸OH in the ground $\Pi_{3/2} J = 5/2 \rightarrow 3/2$ transition, which favors the $J = 5/2^+$ sublevel where the 85.1 μ m component arises. Since collisions with ortho-H₂ quench the asymmetry, the gas is not very warm but should be dense enough so that collisional excitation with para-H₂ competes efficiently with the excitation induced by the radiation field. The asymmetry is not observed in the main isotopologue (Fig. 6e), indicating that either the higher column of OH efficiently mixes the populations of the sublevels, or that OH is tracing warmer gas with increased contribution by collisions with ortho-H₂. However, our model with $n_{\text{H}_2} = 5 \times 10^5$ cm⁻³ and $T_g = 150$ K does not reproduce it, and several tests with higher density and lower T_g were also unsuccessful. Further, since the ground-state ¹⁸OH 120 μ m doublet is not reproduced with the warm component alone, additional absorption by the C_{extended} and C_{halo} components described below, with the same ¹⁶OH-to-¹⁸OH ratio of 70, is included (Fig. 8c).

3.2.4. HCN

Our models for the western nucleus of Arp 220 can also reproduce the fluxes of the HCN lines reported by Rangwala et al. (2011) and the $J = 18 \rightarrow 17$ and $J = 19 \rightarrow 18$ lines detected with PACS (Figs. 9 and 15). For HCN, both collisional excitation and absorption of far-IR photons in the highest-lying lines are required to reproduce the observations. At long wavelengths (i.e. relatively low- J lines), collisional excitation in a warm and dense region is the primary excitation mechanism. For moderate dust opacities, these lines would be detected in emission above the continuum. If collisions are able to excite the molecules up to the rotational level where the dust emission becomes optically thick and the far-IR radiation becomes strong, absorption of far-IR photons in high- J lines continues to excite the molecule to higher-lying levels and the corresponding HCN lines are observed in absorption. Thus the transition from emission to absorption lines is a measure of the dust opacity and temperature of this component, and the high-lying HCN lines detected in absorption are tracing high far-IR radiation densities as well as a warm-dense environment with high HCN column densities.

A grid of models were generated by varying n_{H_2} in the range 10^5 – 3×10^6 cm⁻³ and T_g between 110 and 250 K. For each value of $n_{\text{H}_2} - T_g$, both N_{HCN} and f_C were varied to fit the observed SLED. In all these models, $T_d = 110$ K was adopted. As discussed in Sect. 3.2.1, the high excitation HCN lines can be formed deeper into the dusty, continuum source than lines from other species (Fig. 17), and we extend our HCN shell up to a depth of $\tau_{50} = 4$. Rates for HCN collisions with He were taken from Dumouchel et al. (2010), and scaled for the reduced mass of the HCN-H₂ system to obtain the expected collisional rates with H₂. Our most plausible results were found for $n_{\text{H}_2} = (4\text{--}8) \times 10^5$ cm⁻³ and $T_g \sim 150$ K, for which $N_{\text{HCN}} = (6\text{--}4) \times 10^{17}$ cm⁻², respectively. N_{HCN} is twice these values for $T_g = 110$ K. Decreasing n_{H_2} below 2×10^5 cm⁻³ would involve HCN columns above 10^{18} cm⁻², implying extreme HCN abundances above 2.5×10^{-6} that we consider unlikely. The increase of n_{H_2} above 10^6 cm⁻³ involves lower HCN columns, but the relative absorption in the $J = 12 \rightarrow 11$ line becomes somewhat underpredicted and the value of f_C (or the size of the continuum source) is above that derived for H₂O. Results for $T_g = 150$ K and $n_{\text{H}_2} = 4 \times 10^5$ cm⁻³, with the resulting $N_{\text{HCN}} = 5.6 \times 10^{17}$ cm⁻², are shown in Figs. 9 and 15. The involved far-IR continuum source has the same size as for H₂O and OH. Similar values of $N_{\text{HCN}} = (3\text{--}6) \times 10^{17}$ cm⁻² are obtained for $T_d = 130$ – 90 K, though the sizes of the continuum and HCN sources are in these cases higher and lower than for $T_d = 110$ K, respectively, and similar to those found for H₂O and OH.

In our most plausible models, the HCN/H₂O ratio is 0.1–0.4 (Table 2), and $\chi_{\text{HCN}} = (1\text{--}2) \times 10^{-6}$. In Fig. 15, the calculated HCN SLED is compared with results for a model that neglects the radiative excitation by dust (dotted curve), showing that the dust has a flattening effect on the predicted SLED. Less than 10% of the total column is stored in levels associated with the observed lines; the highest populated levels are $J = 5, 6$. Nevertheless, owing to the high continuum opacity and dust temperature in the nuclear region, as well as to self-absorption in the outermost shells of the HCN region, all HCN lines above $J = 6 \rightarrow 5$ are predicted in absorption. The emission in the $J = 6 \rightarrow 5$ line (Rangwala et al. 2011) is not reproduced, probably indicating that the line is formed in a colder and more extended region associated with relatively weak continuum. On the other hand, the model in Fig. 15 accounts for the observed absorption up to $J = 19 \rightarrow 18$ but fails to explain the absorption coincident with the $J = 21 \rightarrow 20$ transition at 161.3 μ m. If this feature is due to HCN, a region as warm as that proposed for NGC 4418 (Sect. 3.4.1) would be involved.

Our models also include the HCN excitation through the pumping of the vibrationally excited $\nu_2 = 1^1$ state, but we find the effect negligible for the ground-vibrational state lines. Evidently, this is a consequence of the low T_d used in our modeling. Rangwala et al. (2011) have proposed that the pumping of the $\nu_2 = 1^1$ state dominates the HCN excitation, requiring a dust temperature of $T_d > 350$ K. If not completely extinguished, this hot component would show up at mid-IR wavelengths, and there is indeed a hot component (C_{hot}) in our continuum modeling with $T_d = 400$ K (yellow curve in Fig. 1b) attenuated by $A_V \approx 60$ mag, which yields an unattenuated flux at 14 μ m of ≈ 2 Jy -twice as observed. However, C_{hot} has an effective diameter of only ≈ 5 pc, while the observed HCN absorption must be produced over spatial scales of ~ 100 pc because, otherwise, the far-IR HCN absorption would be negligible. Thus, if the HCN molecules are exposed to the radiation of C_{hot} , this

radiation will be diluted and it remains unclear if it can significantly affect the populations. As [Rangwala et al. \(2011\)](#) suggest, the alternative is that there is a hot component much more prominent, but very extinguished, in such a way that it does not show up in the observed SED. The occurrence of this component is plausible, but the HCN molecules responsible for the absorption are in front of, and thus apparently exposed to the non-diluted, unextinguished radiation field characterized by a “moderate” T_d in the range 90–130 K for C_{west} , as the continuum models indicate. The associated dust is very likely optically thick at 14 μm and thus would obscure the emission from the above buried hot component. Our models for the nuclear region are, however, structureless, and more refined models are required to clarify the role of the $\nu_2 = 1^1$ pumping for these lines. Finally, we note that our derived HCN column is a factor of 20 higher than that derived by [Lahuis et al. \(2007\)](#) from the 14 μm absorption band; as the authors state, however, their analysis is based on a covering factor of unity of the mid-IR continuum and their columns are then lower limits.

3.2.5. NH_3

Our model for NH_3 is shown with red lines in Fig. 10 and uses the same parameters as for HCN: $n_{\text{H}_2} = 4 \times 10^5 \text{ cm}^{-3}$, $T_g = 150 \text{ K}$, $T_d = 110 \text{ K}$, and the same source size. The model treats line overlaps, and uses the collisional rates from [Danby et al. \(1988\)](#). The derived column density per unit of τ_{50} is $N_{\text{NH}_3} \approx 1.5 \times 10^{17} \text{ cm}^{-2}$, i.e. $\text{HCN}/\text{NH}_3 \sim 4$ and $\chi_{\text{NH}_3} \approx 4 \times 10^{-7}$. The best fit for all lines is found for $T_g = 150 \text{ K}$, as for $T_g = 250 \text{ K}$ the lower-lying ($3, K$) \rightarrow ($2, K$) lines would be underestimated. There is still some missing flux in these lines at $T_g = 150 \text{ K}$, indicating possible low-level absorption in a more extended region. Within a given K -ladder, excitation through absorption of far-IR photons dominates over collisional excitation. The data are consistent with an ortho-to-para ratio of 1, indicating a formation temperature of at least $\sim 30 \text{ K}$ ([Takano et al. 2000](#)). Similar columns are obtained for $T_d = 90$ and 130 K , with the appropriate source sizes as derived for H_2O , OH , and HCN. Half of the derived NH_3 column is stored in the metastable ($J = K$) levels, giving $\tau_{50} = 1$ metastable columns in agreement with the value inferred by [Ott et al. \(2011\)](#) from the inversion lines for $T_{\text{ex}} = 50 \text{ K}$ ($N_{\text{NH}_3} = 0.84 \times 10^{17} \text{ cm}^{-2}$).

3.3. The low-lying lines in Arp 220: the extended and halo components (C_{extended} and C_{halo})

3.3.1. H_2O

In Arp 220, the absorption in the low-lying $3_{21} \rightarrow 2_{12}$ (Fig. 3k), $2_{21} \rightarrow 1_{10}$ (Fig. 4b), $3_{03} \rightarrow 2_{12}$ (Fig. 4p), and especially the ground-state $2_{12} \rightarrow 1_{01}$ (Fig. 4q) lines, require a more extended, low-excitation region (C_{extended} , G-A04). This is consistent with the continuum models, as the nuclei cannot account for the bulk of the far-IR emission between 50 and 300 μm , and an extended component heated in part by radiation from the nuclei, but with a possible contribution from extended star formation, is invoked (green curve in Fig. 1b). In our models, T_d in C_{extended} is calculated from the balance between heating (by the far-IR emission from the nuclei) and radiative cooling, attaining values between 40 and 90 K. In the model, C_{extended} extends up to an uncertain diameter of $d_{\text{extended}} = 650 \text{ pc}$, has a column of $N_{\text{H}} \sim 8 \times 10^{23} \text{ cm}^{-2}$, an average density of $n_{\text{H}} \sim 10^3 \text{ cm}^{-3}$, and a mass of $M \sim 3 \times 10^9 M_{\odot}$ (Table 1). Most of its luminosity

($\approx 7 \times 10^{11} L_{\odot}$) is likely reemission, rather than intrinsically generated.

With $N_{\text{H}_2\text{O}} = 3 \times 10^{16} \text{ cm}^{-2}$ and $\chi_{\text{H}_2\text{O}} \approx 4 \times 10^{-8}$, the H_2O line absorption due to C_{extended} is shown with green curves in Figs. 3 and 4 only for the lines mentioned above. We have used for this component a “mixed” approach (i.e. dust and molecules coexist) because of the moderate far-IR opacities. We expect reemission in the $3_{03} \rightarrow 2_{12}$ and $3_{22} \rightarrow 3_{13}$ lines (G-A04); in the former line reemission is indeed observed but redshifted (Sect. 2). On the other hand, a transition zone between the nuclear region and C_{extended} is traced by the H_2O lines in emission at $\lambda > 200 \mu\text{m}$ detected by [Rangwala et al. \(2011\)](#), as will be discussed in a future paper.

The depth of the ground-state $2_{12} \rightarrow 1_{01}$ H_2O line at 179.5 μm , however, is not quite reproduced even with the absorption by C_{extended} . The line is probably contaminated by CH^+ ($2 \rightarrow 1$), but its contribution is not expected to completely fill the observed absorption. This is not surprising, as foreground low-excitation molecular absorption of the far-IR emission from the nuclei is not included in the calculations of Sect. 3.2. Thus we have also included a low-excitation component, C_{halo} , with no intrinsic continuum but located in front of the nuclei, so that it absorbs the far-IR emission from the nuclei. This was denoted as the “halo” in G-A04, and it is probably a combination of a part of C_{extended} located in the sight line toward the nuclei, together with more widespread, foreground, low-excitation gas. Although, it is likely that C_{halo} is relatively extended due to its low apparent excitation, we note that its extent is not constrained and it could also include gas close to the nuclei. The H_2O column of this component is uncertain due to line saturation, but it is consistent with $N_{\text{H}_2\text{O}} \sim (5\text{--}10) \times 10^{15} \text{ cm}^{-2}$ (Table 2). The absorption in the [O I] 63 μm line (Fig. 11a) is also expected to be produced in low-excitation gas, which we identify with the C_{halo} component. From the observed $W_{\text{eq}} \approx 45 \text{ km s}^{-1}$ (Fig. 14) corrected for the estimated fraction of the nuclear 63 μm continuum (36%), we obtain $N_{\text{O}^0} \sim 2.5 \times 10^{19} \text{ cm}^{-2}$. For an oxygen abundance of $\chi_{\text{O}^0} = 2.5 \times 10^{-4}$ ([Cartledge et al. 2001](#)), C_{halo} is characterized by $N_{\text{H}} \sim 10^{23} \text{ cm}^{-2}$ and $\tau_{25, \text{fgr}} \sim 1$. The corresponding H_2O abundance is $\chi_{\text{H}_2\text{O}} \sim 0.5 \times 10^{-7}$ relative to H nuclei, similar to the value found in Galactic translucent clouds ([Plume et al. 2004](#)). The inferred $N_{\text{H}} \sim 10^{23} \text{ cm}^{-2}$ and 25 μm continuum opacity of ~ 1 are close to the values obtained from the fit to the continuum for the absorbing layer in front of the nuclei and of the hot component (Table 1). While the column density across the C_{halo} component is only accurate within a factor 2, the above comparison suggests that C_{halo} is the origin of the foreground extinction of the mid-IR nuclear emission.

Figure 19b shows the predicted-to-observed flux ratios of the detected lines for the full reference model including C_{west} , C_{east} , and C_{extended} . Values for the contaminated $7_{17} \rightarrow 6_{06}$ and $2_{12} \rightarrow 1_{01}$ lines are not plotted. Only two lines, the $4_{31} \rightarrow 4_{22}$ (147 μm) and $6_{15} \rightarrow 6_{06}$ (104 μm) show departures larger than 50%, but the small predicted-to-observed value of the latter probably indicates that the feature is contaminated by OH^+ (Sect. 2). Among the undetected lines, the absorption in the $5_{33} \rightarrow 4_{22}$ and $4_{13} \rightarrow 4_{04}$ lines at 53.1 and 187.1 μm (Figs. 3a and 4o) are too strong in all relevant models.

3.3.2. OH

The far-IR spectrum of H_2O has only one ground-state line at 179.5 μm . Since this line is strongly saturated, the species is better suited to describe the region of highest molecular excitation.

Table 1. Parameters of the continuum models.

Source	C^a	Diameter (pc)	T_d (K)	τ_d at 200 μm	N_H^b (cm^{-2})	M^c ($10^8 M_\odot$)	L^d (L_\odot)	$\tau_{25,\text{fgr}}^e$	L_{att}^f (L_\odot)
NGC 4418	C_{hot}	5.2	350	0.007	3.5×10^{22}	8×10^{-5}	8.5×10^{10}	1.3	9.0×10^9
	C_{core}	20	140–150	1–2	$(0.5–1) \times 10^{25}$	0.16–0.33	$(6–8) \times 10^{10}$	1.5	3.1×10^{10}
	C_{warm}	31	110	0.5	2.4×10^{24}	0.2	6×10^{10}	1.2	2.9×10^{10}
Arp 220	C_{extended}	200	90–30	0.03	$(1.0–1.3) \times 10^{23}$	0.18	2.4×10^{10}	0	2.4×10^{10}
	C_{hot}	5.2	400	0.007	3.4×10^{22}	8×10^{-5}	1.4×10^{11}	1.1	2.0×10^{10}
	C_{west}	150–80	90–130	6–12	$(3–6) \times 10^{25g}$	55–30 ^g	$(6.5–8.2) \times 10^{11}$	1.4	3.7×10^{11}
	C_{east}	108	87	2.7	1.3×10^{25}	13	3×10^{11}	1.0	2.1×10^{11}
	C_{extended}	650	90–40	0.17	8×10^{23}	30	6.9×10^{11}	0	6.9×10^{11}

Notes. ^(a) Component: in Arp 220, C_{west} (C_{east}) is the western (east) nucleus. ^(b) Column density of H nuclei, calculated assuming a mass-absorption coefficient of $12.3 \text{ cm}^2/\text{g}$ at $200 \mu\text{m}$ and a gas-to-dust mass ratio of 100. ^(c) Estimated mass, assuming spherical symmetry. ^(d) Unattenuated luminosity of the component. ^(e) Foreground opacity at $25 \mu\text{m}$. ^(f) Attenuated luminosity of the component. ^(g) The estimated mass of C_{west} , based on the flux density at $860 \mu\text{m}$ reported by Sakamoto et al. (2008) and on an emissivity index of $\beta = 2$ in the submillimeter ($\kappa_{860} \approx 0.7 \text{ cm}^2 \text{ g}^{-1}$ of dust), is higher than the dynamical mass of $\sim 10^9 M_\odot$ estimated by several authors (Downes & Solomon 1998; Sakamoto et al. 2008). This probably indicates that $\beta = 1$ is a better approach in the submillimeter (yielding $\kappa_{860} \sim 3 \text{ cm}^2 \text{ g}^{-1}$ of dust), as estimated for some Galactic massive star-forming regions (e.g. Zhang et al. 2007).

Table 2. Derived H_2O column densities and abundances, column density ratios, and covering factors of the continua.

Source	C^a	$N_{\text{H}_2\text{O}}^b$ (cm^{-2})	$\chi_{\text{H}_2\text{O}}^c$	$\text{OH}/\text{H}_2\text{O}^d$	$\text{HCN}/\text{H}_2\text{O}^d$	HCN/NH_3^d	$f_C(\text{H}_2\text{O})^e$	$f_C(\text{OH})^e$	$f_C(\text{HCN}, \text{NH}_3)^e$
NGC 4418	C_{core}	$(2–6) \times 10^{18}$	$(0.5–1.5) \times 10^{-5}$	0.3–0.6	0.1–0.3	2–4	0.85	1	0.7
	C_{warm}	$\sim 5 \times 10^{16}$	$(0.5–2.5) \times 10^{-7}$	~ 0.4			1	1	
	C_{extended}	$\sim 0.2 \times 10^{16}$	$\sim 2 \times 10^{-8}$	5–10			0.45	0.45	
Arp 220	C_{west}	$(0.8–6) \times 10^{18}$	$(0.2–1.5) \times 10^{-5}$	0.4–1.0	0.1–0.4	3–5	0.7–1	0.7–1	0.7–1
	C_{east}	3×10^{17}	0.8×10^{-6}	~ 1			0.4	0.4	
	C_{extended}	3×10^{16}	4×10^{-8}	~ 3			1	1	
	C_{halo}	$(5–10) \times 10^{15}$	5×10^{-8}	~ 10			0.7	1	

Notes. ^(a) Component (see Table 1). In Arp 220, C_{halo} is an absorbing, widespread component in front of the nuclear region. ^(b) Column densities per unit of dust opacity at $50 \mu\text{m}$, τ_{50} , for C_{core} and C_{warm} in NGC 4418, and for C_{west} and C_{east} in Arp 220, with an estimated column of H nuclei per τ_{50} of $4 \times 10^{23} \text{ cm}^{-2}$. For the C_{extended} component in both sources, mixed values (i.e., dust and molecules are coexistent throughout the source; see text for details). ^(c) Estimated H_2O abundance relative to H nuclei. ^(d) Column density ratios. ^(e) Covering factor of the continuum (same value for HCN and NH_3).

OH has, however, within the PACS wavelength coverage three ground-state doublets with different strengths at 119, 79, and $53.3 \mu\text{m}$ (Fig. 2), allowing us to better characterize the C_{extended} and C_{halo} components. This is illustrated in Figs. 6a–c, where the highly excited OH in the nuclei is expected to produce weak absorption in these ground-state lines, thus requiring a more extended region where relatively low-excited OH absorbs a significant fraction of the far-IR continuum of the galaxy. Two more OH transitions also trace C_{extended} : the $\Pi_{3/2} 7/2 \rightarrow 5/2$ doublet at $84 \mu\text{m}$ (Fig. 6e), and the $\Pi_{1/2} 3/2 \rightarrow 1/2$ doublet at $163 \mu\text{m}$. The former line, with $E_{\text{lower}} = 120 \text{ K}$, is also too strong to be reproduced with the model for the nuclei, and should be significantly excited in C_{extended} . The $163 \mu\text{m}$ doublet, the only one observed in emission, is excited in C_{extended} through absorption of continuum photons in the ground-state 53.3 and $35 \mu\text{m}$ lines, followed by cascade down to the ground OH state (Genzel et al. 1985), and thus traces large spatial-scale gas illuminated by the strong far-IR continuum (G-A04). We indeed expect the $163 \mu\text{m}$ doublet to be in absorption toward the nuclei (Fig. 6j), and thus C_{extended} is required to produce emission in the line. The above pumping mechanism also has observational effects on the ground-state $79 \mu\text{m}$ line: since every $163 \mu\text{m}$ photon should be accompanied, through downward cascade, by a $79 \mu\text{m}$ line photon, the emission in the $163 \mu\text{m}$ doublet ensures emission in the $79 \mu\text{m}$ transition as well. This is indeed observed in Arp 220

(Figs. 6b and 11d), where the $79 \mu\text{m}$ doublet shows an emission feature at the most redshifted velocities of 300 km s^{-1} with respect to the systemic one; at lower velocities, one would expect a combination of emission and absorption with the latter dominating for suitable geometries and/or sufficiently large amounts of OH in front of the far-IR continuum source. With $163 \mu\text{m}$ absorption in front of the nuclei, and emission from more extended regions, the $163 \mu\text{m}$ doublet is expected to be redshifted in outflowing gas, as observed in Arp 220 (Fig. 6j).

In our specific model for Arp 220, the required OH column and abundance in C_{extended} are $N_{\text{OH}} \approx 10^{17} \text{ cm}^{-2}$ and $\chi_{\text{OH}} \approx 1.3 \times 10^{-7}$, much lower than towards the nuclear region and favoring an OH/ H_2O column ratio of ~ 3 . This ratio reverses the value found in the nuclear region where OH/ H_2O is ~ 0.5 . The C_{extended} component then accounts for the $163 \mu\text{m}$ line, though the redshift is not reproduced as no outflow is included in this component, and for the absorption at $84 \mu\text{m}$. Similar to H_2O , however, the full absorption in the ground-state 119, 79, and $53.3 \mu\text{m}$ doublets is not reproduced; in particular, the absorption in the $79 \mu\text{m}$ line is predicted to be very weak. We again find that the missing absorption can be attributed to C_{halo} , requiring a column of $N_{\text{OH}} \sim 8 \times 10^{16} \text{ cm}^{-2}$. The contribution of this component to the absorption in the ground-state 119, 79, and $53.3 \mu\text{m}$ doublets is shown with yellow curves in Figs. 6a–c. The OH/ H_2O column density ratio in C_{halo} is estimated to be ~ 10 , but

Table 3. H₂O line equivalent widths, fluxes, and velocity shifts.

Line	λ (μm)	W_{eq}^a (km s^{-1})	NGC 4418		W_{eq}^a (km s^{-1})	Arp 220	
			flux ^a ($10^{-21} \text{ W cm}^{-2}$)	$V_{\text{shift}}^{a,b}$ (km s^{-1})		flux ^a ($10^{-21} \text{ W cm}^{-2}$)	$V_{\text{shift}}^{a,b}$ (km s^{-1})
H ₂ O 5 ₃₃ → 4 ₂₂	53.138	24.9(6.5)	-20.0(5.2)	35(29)	1.9(2.6)	-4.5(6.3)	
H ₂ O 8 ₂₇ → 7 ₁₆ ^c	55.131	6.2(2.3)	-4.8(1.8)	-3(16)			
H ₂ O 4 ₃₁ → 3 ₂₂	56.325	35.6(1.8)	-26.6(1.4)	-8(33)	30.0(1.2)	-65.3(2.6)	-29(49)
H ₂ O 4 ₂₂ → 3 ₁₃	57.636	37.1(2.1)	-28.0(1.5)	-15(35)	22.8(1.3)	-49.3(2.8)	14(43)
H ₂ O 4 ₃₂ → 3 ₂₁	58.699	50.7(0.9)	-37.8(0.7)	16(34)	34.7(1.0)	-74.9(2.1)	-87(47)
H ₂ O 7 ₂₆ → 6 ₁₅ ^c	59.987	5.6(1.3)	-4.1(1.0)	-6(22)			
H ₂ O 4 ₃₁ → 4 ₀₄	61.809	11.1(2.6)	-7.3(1.7)	37(24)	2.3(1.4)	-4.9(3.0)	
H ₂ O 8 ₁₈ → 7 ₀₇	63.324	13.3(1.0)	-9.1(0.7)	33(18)	2.4(0.6)	-5.1(1.3)	
H ₂ O 7 ₁₆ → 6 ₂₅	66.093	11.8(0.9)	-7.5(0.6)	-6(24)	5.7(1.0)	-12.3(2.1)	
H ₂ O 3 ₃₀ → 2 ₂₁	66.438	64.7(1.3)	-41.8(0.9)	-18(34)	40.8(0.8)	-87.8(1.8)	-55(38)
H ₂ O 3 ₃₁ → 2 ₂₀	67.089	43.6(2.2)	-28.1(1.4)	12(31)	41.6(0.9)	-90.4(2.1)	-30(49)
H ₂ O 3 ₃₀ → 3 ₀₃	67.269	13.2(1.3)	-8.5(0.8)	-9(29)	7.7(2.3)	-16.7(4.9)	-24(51)
H ₂ O 5 ₂₄ → 4 ₁₃	71.067	23.9(1.7)	-13.6(1.0)	-45(24)	16.7(1.0)	-33.2(2.0)	35(44)
H ₂ O 7 ₁₇ → 6 ₀₆	71.540	17.6(1.8)	-9.7(1.0)	27(34)	9.5(0.8)	-19.0(1.6)	
H ₂ O 7 ₀₇ → 6 ₁₆	71.947	25.5(2.3)	-13.8(1.2)	-11(32)	10.0(0.8)	-20.1(1.7)	35(38)
H ₂ O 7 ₂₅ → 6 ₃₄ ^c	74.945	5.0(1.5)	-2.6(0.8)	-15(23)			
H ₂ O 3 ₂₁ → 2 ₁₂	75.381	73.9(1.1)	-38.6(0.6)	-23(32)	79.7(0.8)	-153.4(1.6)	4(41)
H ₂ O 4 ₂₃ → 3 ₁₂	78.742	40.3(1.9)	-19.1(0.9)	-36(27)	34.4(0.9)	-62.9(1.6)	-42(43)
H ₂ O 6 ₁₅ → 5 ₂₄	78.928	19.4(1.8)	-9.3(0.9)	-4(27)	4.9(0.8)	-8.8(1.4)	-70(31)
H ₂ O 6 ₁₆ → 5 ₀₅	82.031	31.4(1.4)	-14.1(0.6)	2(25)	20.3(0.6)	-35.6(1.1)	-21(37)
H ₂ O 6 ₀₆ → 5 ₁₅	83.284	25.1(1.7)	-11.3(0.7)	-16(27)	16.1(1.2)	-27.5(2.0)	-4(41)
H ₂ O 3 ₂₂ → 2 ₁₁	89.988	60.4(1.7)	-23.3(0.7)	5(27)	39.8(1.1)	-60.6(1.6)	-32(35)
H ₂ O 6 ₄₃ → 6 ₃₄ ^c	92.811	8.0(1.6)	-3.0(0.6)	-35(19)			
H ₂ O 6 ₂₅ → 6 ₁₆	94.644	10.1(1.7)	-3.6(0.6)	-37(17)			
H ₂ O 4 ₄₁ → 4 ₃₂	94.705	14.3(1.8)	-5.1(0.6)	-33(18)			
H ₂ O 5 ₁₅ → 4 ₀₄	95.627	42.9(2.4)	-15.2(0.8)	-11(30)	22.8(2.1)	-31.6(2.9)	9(41)
H ₂ O 4 ₄₀ → 4 ₃₁	95.885	12.5(2.0)	-4.3(0.7)	-2(20)	3.0(1.7)	-4.1(2.3)	
H ₂ O 6 ₁₅ → 6 ₀₆ ^d	103.940	10.0(1.4)	-2.9(0.4)	68(29)	7.6(1.4)	-9.5(1.7)	-34(42)
H ₂ O 2 ₂₁ → 1 ₁₀	108.073	67.4(2.6)	-17.5(0.7)	-23(46)	72.2(2.1)	-82.9(2.4)	40(47)
H ₂ O 5 ₂₄ → 5 ₁₅	111.628	24.8(2.2)	-6.1(0.5)	42(55)	4.2(0.7)	-4.5(0.8)	
H ₂ O 4 ₁₄ → 3 ₀₃	113.537	36.7(2.1)	-8.5(0.5)	14(39)	26.0(2.9)	-27.0(3.1)	-32(44)
H ₂ O 4 ₀₄ → 3 ₁₃	125.354	25.4(1.8)	-4.6(0.3)	-19(33)	27.7(1.2)	-23.7(1.0)	-6(54)
H ₂ O 3 ₃₁ → 3 ₂₂ ^d	126.714	12.0(1.8)	-2.1(0.3)	55(35)	8.8(5.3)	-7.4(4.4)	14(119)
H ₂ O 4 ₂₃ → 4 ₁₄	132.408	28.1(2.5)	-4.6(0.4)	5(68)	12.6(0.8)	-9.7(0.6)	-29(46)
H ₂ O 5 ₁₄ → 5 ₀₅	134.935	26.1(1.9)	-4.1(0.3)	0(49)	8.6(0.8)	-6.3(0.6)	18(40)
H ₂ O 3 ₃₀ → 3 ₂₁	136.496	36.9(1.9)	-5.5(0.3)	0(46)	19.8(0.8)	-14.3(0.6)	-37(48)
H ₂ O 3 ₁₃ → 2 ₀₂	138.528	30.7(1.4)	-4.5(0.2)	30(39)	29.0(1.2)	-20.2(0.8)	-40(45)
H ₂ O 4 ₁₃ → 3 ₂₂	144.518	11.9(1.7)	-1.5(0.2)	-32(28)	11.6(0.9)	-7.3(0.6)	-24(40)
H ₂ O 4 ₃₁ → 4 ₂₂	146.923	12.2(2.1)	-1.5(0.3)	-17(33)	3.3(0.6)	-2.0(0.3)	-23(27)
H ₂ O 3 ₂₂ → 3 ₁₃	156.194	9.2(2.3)	-1.0(0.2)	30(26)	14.5(0.9)	-7.5(0.5)	-29(38)
H ₂ O 3 ₀₃ → 2 ₁₂	174.626	13.2(2.5)	-1.0(0.2)	-7(15)	20.3(3.7)	-7.3(1.3)	-33(26)
H ₂ O 2 ₁₂ → 1 ₀₁ ^d	179.527	81.9(4.9)	-5.5(0.3)	118(35)	167.3(5.1)	-51.5(1.6)	34(40)

Notes. ^(a) Numbers in parenthesis indicate 1σ uncertainties from Gaussian fits to the lines. ^(b) Velocity shifts are relative to $z = 0.00705$ for NGC 4418 and $z = 0.0181$ for Arp 220. ^(c) Marginal detection. ^(d) Probably contaminated.

the relative OH and H₂O columns in the C_{extended} and C_{halo} components are uncertain due to the difficulty of disentangling the two components.

The ground-state $35 \mu\text{m}$ doublet of OH ($\Pi_{1/2} \rightarrow \Pi_{3/2} 5/2 \rightarrow 3/2$) has been observed with ISO by Skinner et al. (1997); correcting their continuum flux density at $35 \mu\text{m}$ (62 Jy) to the lower value of 40 Jy indicated by the *Spitzer* IRS spectrum in Fig. 1b, the observed absorbing flux in the $35 \mu\text{m}$ doublet is $\approx 1.3 \times 10^{-12} \text{ erg s}^{-1} \text{ cm}^{-2}$. The joint contribution of C_{west} , C_{east} , C_{extended} , and C_{halo} predicts a comparable absorbing flux of $\approx 1.1 \times 10^{-12} \text{ erg s}^{-1} \text{ cm}^{-2}$, dominated by C_{halo} (G-A04).

3.4. The high-lying lines in NGC 4418: the nuclear core (C_{core})

3.4.1. HCN and H₂O

Similar to Arp 220, NGC 4418 shows strong mid-IR silicate absorption (Fig. 1, see also Spoon et al. 2001) and absorption in the [O I] $63 \mu\text{m}$ line, indicating important mid-IR extinction. We have thus followed a similar analysis as for Arp 220, based on the combination of the continuum and line absorption. In NGC 4418, line broadening is purely modeled as microturbulence with $v_{\text{tur}} = 60 \text{ km s}^{-1}$.

Table 4. [O I] and OH line equivalent widths, fluxes, and velocity shifts.

Line	λ (μm)	W_{eq}^a (km s^{-1})	NGC 4418		Arp 220		
			Flux ^a ($10^{-21} \text{ W cm}^{-2}$)	$V_{\text{shift}}^{a,b}$ (km s^{-1})	W_{eq}^a (km s^{-1})	Flux ^a ($10^{-21} \text{ W cm}^{-2}$)	$V_{\text{shift}}^{a,b}$ (km s^{-1})
[O I] 1–2	63.184	25.2(1.0)	–17.2(0.7)	115(16)	45.4(2.0)	–96.3(4.3)	20(30)
[O I] 0–1	145.525	–7.3(1.6)	0.9(0.2)	35(22)	–25.4(1.1)	15.6(0.7)	75(77)
OH $\Pi_{3/2} - \Pi_{3/2}$	119.233	58.4(2.0)	–12.0(0.4)	125(36)	212.5(2.2)	–204.5(2.1)	41(52)
OH $\Pi_{3/2} - \Pi_{3/2}$	119.441	54.9(1.9)	–11.2(0.4)	114(32)	174.9(2.0)	–168.1(1.9)	39(44)
OH $\Pi_{1/2} - \Pi_{3/2}$	79.118	17.8(1.4)	–8.7(0.7)	97(24)	63.5(1.3)	–115.0(2.3)	90(35)
OH $\Pi_{1/2} - \Pi_{3/2}$	79.181	12.5(1.3)	–6.1(0.6)	72(19)	63.5(1.3)	–115.0(2.3)	90(35)
OH $\Pi_{1/2} - \Pi_{3/2}$	53.261	38.8(4.5)	–31.3(3.6)	76(35)	95.7(3.8)	–230.5(9.1)	66(44)
OH $\Pi_{1/2} - \Pi_{3/2}$	53.351	59.2(5.6)	–47.7(4.5)	56(52)	94.4(3.7)	–227.3(8.8)	31(42)
OH $\Pi_{1/2} - \Pi_{3/2}$	96.340	9.1(3.3)	–3.1(1.1)	38(34)			
OH $\Pi_{3/2} - \Pi_{3/2}$	84.420	77.8(1.9)	–34.2(0.8)	10(30)	88.6(1.4)	–150.8(2.3)	2(38)
OH $\Pi_{3/2} - \Pi_{3/2}$	84.597	89.6(2.0)	–39.2(0.9)	1(34)	95.4(1.4)	–161.7(2.3)	–16(39)
OH $\Pi_{3/2} - \Pi_{3/2}$	65.132	74.1(1.7)	–48.7(1.1)	16(39)	49.8(1.2)	–107.7(2.6)	–6(50)
OH $\Pi_{3/2} - \Pi_{3/2}$	65.279	62.7(1.8)	–40.8(1.1)	–13(39)	45.8(1.2)	–98.8(2.5)	–57(49)
OH $\Pi_{1/2} - \Pi_{1/2}$	71.197	72.1(2.8)	–40.5(1.6)	–16(45)	42.4(1.0)	–84.3(2.0)	–17(54)
OH $\Pi_{3/2} - \Pi_{3/2}$	52.934	24.1(5.0)	–18.8(3.9)	–57(22)	3.0(2.2)	–7.4(5.5)	–67(40)
OH $\Pi_{3/2} - \Pi_{3/2}$	53.057	23.5(5.4)	–18.5(4.3)	91(25)	3.6(3.8)	–8.8(9.3)	4(33)
OH $\Pi_{1/2} - \Pi_{1/2}$	55.920	54.1(4.4)	–41.0(3.3)	40(91)	12.5(2.5)	–26.9(5.4)	–52(58)
OH $\Pi_{1/2} - \Pi_{1/2}$	163.124	–10.0(2.2)	1.0(0.2)	–78(24)	–71.9(2.7)	31.9(1.2)	150(77)
OH $\Pi_{1/2} - \Pi_{1/2}$	163.397	–9.6(2.2)	0.9(0.2)	–16(23)	–41.8(5.0)	18.5(2.2)	161(57)

Notes. ^(a) Numbers in parenthesis indicate 1σ uncertainties from Gaussian fits to the lines. ^(b) Velocity shifts are relative to $z = 0.00705$ for NGC 4418 and $z = 0.0181$ for Arp 220. ^(c) The two Λ -components are (nearly) blended into a single spectral feature.

Table 5. HCN line equivalent widths, fluxes, and velocity shifts.

Line	λ (μm)	W_{eq}^a (km s^{-1})	NGC 4418		Arp 220		
			Flux ^a ($10^{-21} \text{ W cm}^{-2}$)	$V_{\text{shift}}^{a,b}$ (km s^{-1})	W_{eq}^a (km s^{-1})	Flux ^a ($10^{-21} \text{ W cm}^{-2}$)	$V_{\text{shift}}^{a,b}$ (km s^{-1})
HCN 25 \rightarrow 24	135.626	5.8(1.8)	–0.9(0.3)	–20(43)			
HCN 23 \rightarrow 22	147.365	9.4(1.9)	–1.1(0.2)	69(23)			
HCN 22 \rightarrow 21	154.037	12.3(1.6)	–1.3(0.2)	19(35)	4.3(2.0)	–2.3(1.1)	–35(58)
HCN 21 \rightarrow 20 ^c	161.346	14.7(2.7)	–1.5(0.3)	7(21)	9.6(1.5)	–4.5(0.7)	–53(45)
HCN 20 \rightarrow 19	169.386	12.7(2.7)	–1.0(0.2)	–6(20)			
HCN 19 \rightarrow 18	178.274	11.0(3.8)	–0.8(0.3)	21(27)	3.8(2.0)	–1.2(0.6)	24(72)
HCN 18 \rightarrow 17	188.151	21.0(5.4)	–0.9(0.2)	–16(20)	15.2(3.2)	–3.1(0.6)	–100(37)

Notes. ^(a) Numbers in parenthesis indicate 1σ uncertainties from Gaussian fits to the lines. ^(b) Velocity shifts are relative to $z = 0.00705$ for NGC 4418 and $z = 0.0181$ for Arp 220. ^(c) Doubtful identification in Arp 220.

The extreme excitation of H₂O and HCN provides the most stringent requirements for the dust temperature (T_d), gas temperature (T_g), density (n_{H_2}), and column densities in the nuclear region. The high-lying lines of these species arise in a compact component that we denote as the “nuclear core” (C_{core}). Preliminary models for HCN in the C_{core} component of NGC 4418 are shown in Figs. 9 and 15, with the HCN shell extended up to a depth of $\tau_{50} = 4$. We generated several models that included/excluded excitation through collisions, absorption of far-IR radiation, and pumping through the $\nu_2 = 1^1$ state, and found that HCN is primarily excited through collisions, with the far-IR emission significantly modifying the distribution of populations in the highest lines. With the SLED apparently peaking at $J = 21 \rightarrow 20$, the C_{core} model requires $n_{\text{H}_2} \sim 3 \times 10^6 \text{ cm}^{-3}$ and T_g in the most probable range of 220–250 K, significantly higher than in Arp 220. Decreasing n_{H_2} by a factor of 2 would

increase T_g to ≈ 300 K. The high density and T_g values are also required to reduce the otherwise too strong OH absorption in the ground-state lines, to account for the NH₃ observations described below, and to reproduce the far-IR CO emission (discussed in a forthcoming paper). In spite of the high collisional excitation, the HCN lines are detected in absorption, indicating that the dust in C_{core} is warm and at least a fraction of C_{core} is optically thick at far-IR wavelengths. A reasonable fit to the HCN lines is obtained with $T_d = 140\text{--}150$ K and $\tau_{200} \gtrsim 1$ for the continuum. With $\tau_{200} \approx 1$ (solid curve and triangles in Fig. 15), we expect the rotational lines $J_{\text{upper}} \leq 14$ to be in emission. The strength of the emission lines would decrease if $\tau_{200} \approx 4$ (dashed curve), and further weaken with a screen model for HCN (dotted curve). The inferred HCN column per unit of τ_{50} is $N_{\text{HCN}} = (6\text{--}7.5) \times 10^{17} \text{ cm}^{-2}$, i.e. $\chi_{\text{HCN}} = (1.5\text{--}2) \times 10^{-6}$. As for Arp 220, we find that the pumping of the $\nu_2 = 1^1$ state has

Table 6. NH₃ line equivalent widths and fluxes for relatively isolated spectral features.

Line	λ (μm)	NGC 4418		Arp 220	
		W_{eq}^a (km s^{-1})	Flux ^a ($10^{-21} \text{ W cm}^{-2}$)	W_{eq}^a (km s^{-1})	Flux ^a ($10^{-21} \text{ W cm}^{-2}$)
NH ₃ (8, 6) <i>s</i> → (7, 6) <i>a</i>	62.888	3.9(1.7)	-2.7(1.1)		
NH ₃ (7, 6) <i>a</i> → (6, 6) <i>s</i>	72.439	6.7(0.6)	-3.6(0.3)	4.6(0.5)	-9.2(1.0)
NH ₃ (6, 5) <i>s</i> → (5, 5) <i>a</i>	83.432	10.1(1.2)	-4.5(0.5)	4.5(0.8)	-7.6(1.4)
NH ₃ (6, 4) <i>s</i> → (5, 4) <i>a</i>	83.590	13.6(1.4)	-6.1(0.6)	^b	^b
NH ₃ (6, 3) <i>s</i> → (5, 3) <i>a</i>	83.709	10.1(1.0)	-4.5(0.5)	3.0(0.7)	-5.1(1.1)
NH ₃ (6, 2) <i>s</i> → (5, 2) <i>a</i>	83.794	4.5(1.0)	-2.0(0.4)	^b	^b
NH ₃ (6, 1-0) <i>s</i> → (5, 1-0) <i>a</i> ^c	83.844–83.861	11.0(1.1)	-4.9(0.5)	7.5(1.2)	-12.9(2.1)
NH ₃ (4, 3) <i>s</i> → (3, 3) <i>a</i>	124.648	17.9(1.7)	-3.3(0.3)	25.1(1.1)	-21.6(0.9)
NH ₃ (4, 2-1-0) <i>s</i> → (3, 2-1-0) <i>a</i> ^c	124.796–124.913	38.3(1.6)	-7.0(0.3)	21.5(1.2)	-18.5(1.1)
NH ₃ (4, 3-2-1) <i>a</i> → (3, 3-2-1) <i>s</i> ^c	127.108–127.181	38.9(1.3)	-6.9(0.2)	28.9(0.9)	-24.1(0.7)
NH ₃ (3, 2) <i>s</i> → (2, 2) <i>a</i> ^d	165.597	30.9(2.3)	-2.8(0.2)	27.6(2.0)	-11.8(0.9)
NH ₃ (3, 1) <i>s</i> → (2, 1) <i>a</i> ^d	165.729	13.6(2.4)	-1.2(0.2)	^b	^b
NH ₃ (3, 2-1-0) <i>a</i> → (2, 2-1-0) <i>s</i> ^c	169.968–169.996	26.9(3.4)	-2.2(0.3)	33.7(1.5)	-13.2(0.6)

Notes. ^(a) Numbers in parenthesis indicate 1σ uncertainties from Gaussian fits to the lines. ^(b) Uncertain due to baseline subtraction or blending. ^(c) Joint emission of several *K*-lines. ^(d) Probably contaminated by H₃O⁺.

Table 7. H₂¹⁸O line equivalent widths and fluxes.

Line	λ (μm)	NGC 4418		Arp 220	
		W_{eq}^a (km s^{-1})	Flux ^a ($10^{-21} \text{ W cm}^{-2}$)	W_{eq}^a (km s^{-1})	Flux ^a ($10^{-21} \text{ W cm}^{-2}$)
H ₂ ¹⁸ O 4 ₃₂ → 3 ₂₁	59.350	1.5(0.9)	-1.0(0.6)	7.9(1.1)	-17.2(2.5)
H ₂ ¹⁸ O 3 ₃₁ → 2 ₂₀	67.883	2.0(0.9)	-1.2(0.6)	8.3(0.9)	-18.0(1.9)
H ₂ ¹⁸ O 3 ₂₁ → 2 ₁₂	75.867	7.0(1.6)	-3.5(0.8)	17.9(0.8)	-34.7(1.5)
H ₂ ¹⁸ O 4 ₂₃ → 3 ₁₂	79.531	6.0(1.1)	-2.9(0.5)	5.4(0.8)	-9.6(1.4)
H ₂ ¹⁸ O 3 ₂₂ → 2 ₁₁	90.936	3.5(1.5)	-1.3(0.6)	4.2(0.7)	-6.4(1.1)
H ₂ ¹⁸ O 2 ₂₁ → 1 ₁₀	109.347	5.7(1.6)	-1.5(0.4)	13.2(1.8)	-14.8(2.0)
H ₂ ¹⁸ O 4 ₁₄ → 3 ₀₃	114.296	^b	^b	7.0(1.5)	-7.2(1.5)
H ₂ ¹⁸ O 3 ₁₃ → 2 ₀₂	139.586			10.0(0.8)	-6.8(0.5)
H ₂ ¹⁸ O 3 ₀₃ → 2 ₁₂	174.374			7.9(1.5)	-2.9(0.6)
H ₂ ¹⁸ O 2 ₂₁ → 2 ₁₂	183.530			14.8(2.5)	-3.8(0.7)

Notes. ^(a) Numbers in parenthesis indicate 1σ uncertainties from Gaussian fits to the lines. ^(b) Uncertain due to baseline subtraction.

Table 8. ¹⁸OH line equivalent widths and fluxes.

Line	λ (μm)	NGC 4418		Arp 220	
		W_{eq}^a (km s^{-1})	Flux ^a ($10^{-21} \text{ W cm}^{-2}$)	W_{eq}^a (km s^{-1})	Flux ^a ($10^{-21} \text{ W cm}^{-2}$)
¹⁸ OH $\Pi_{3/2} - \Pi_{3/2} \frac{9}{2}^+ - \frac{7}{2}^-$	65.690	1.7(0.9)	-1.1(0.6)	4.9(0.9)	-10.6(1.9)
¹⁸ OH $\Pi_{3/2} - \Pi_{3/2} \frac{7}{2}^+ - \frac{5}{2}^-$	84.947	2.1(0.9)	-0.9(0.4)	7.0(0.8)	-11.8(1.3)
¹⁸ OH $\Pi_{3/2} - \Pi_{3/2} \frac{5}{2}^- - \frac{3}{2}^+$	85.123	0.7(0.7)	-0.3(0.3)	12.9(0.8)	-21.5(1.4)
¹⁸ OH $\Pi_{3/2} - \Pi_{3/2} \frac{5}{2}^+ - \frac{3}{2}^-$	120.171	0.4(0.8)	-0.1(0.2)	38.7(2.2)	-36.7(2.0)

Notes. ^(a) Numbers in parenthesis indicate 1σ uncertainties from Gaussian fits to the lines.

little effect on the excitation and strength of the detected high-*J* ground-vibrational state lines, as expected from our moderate value for T_d (Sakamoto et al. 2010).

The minimum diameter of C_{core} , $d = 16.5$ pc, is obtained by assuming $f_C = 1$. The corresponding luminosity is $\approx 6 \times 10^{10} L_{\odot}$, about 60% of the entire luminosity of the galaxy. The C_{core} component cannot be much bigger or warmer as its luminosity would exceed the bolometric luminosity of the galaxy (assuming spherical symmetry for the emitting radiation). We also attempted

to fit the HCN SLED with lower T_d in the range 110–140 K. At 130 K, the source size is increased by 18% relative to the 150 K case, the C_{core} luminosity is decreased by 20%, and the $J = 25 \rightarrow 24$ line is underestimated; thus our modeling favors $T_d \gtrsim 130$ K. With $T_d = 150$ K, most energy is emitted at wavelengths shorter than 40 μm , but the flux density at 150–190 μm is still 4.5–3 Jy, and this is the continuum absorbed by the HCN. In Fig. 1a, the SED of C_{core} (blue curve), with an adopted $d = 20$ pc, is attenuated by foreground dust

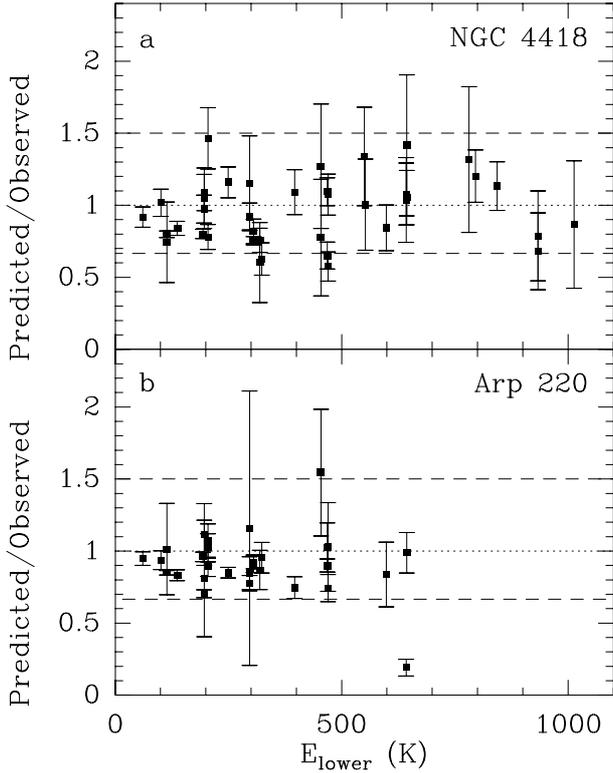


Fig. 19. Predicted-to-observed H₂O flux ratios in NGC 4418 (*upper panel*) and Arp 220 (*lower panel*) for the models including all components. See Sect. 3 for details.

with $\tau_{25,\text{fgr}} = 1.5$. The corresponding covering factor for HCN is $f_C \approx 0.7$. With $\tau_{200} = 1-2$, the radial column through C_{core} is $N_{\text{H}} \sim (0.5-1) \times 10^{25} \text{ cm}^{-2}$, sufficient to strongly attenuate the X-ray emission from an AGN located at the center.

The C_{core} model was applied to H₂O, and results are shown in Figs. 3 and 4 (blue curves). The highest excited H₂O lines are the least saturated ones, which makes them most sensitive to the column density, and we derive $N_{\text{H}_2\text{O}}$ in the range $(3-6) \times 10^{18} \text{ cm}^{-2}$. The H₂O abundance relative to H is as high as $\chi_{\text{H}_2\text{O}} = (0.5-1.5) \times 10^{-5}$, and the corresponding HCN/H₂O ratio in C_{core} is 0.1–0.3. The H₂O models also confirm the very warm ($T_{\text{d}} = 140-150 \text{ K}$) source of far-IR emission, though the dust mixed in the H₂O shell has a somewhat lower $T_{\text{d}} = 130 \text{ K}$ to avoid strong emission in the $6_{24} \rightarrow 6_{15}$ line at $167 \mu\text{m}$ (Fig. 4n). H₂O excitation through collisions has two main effects: first, it increases the excitation of the low-lying lines among the lowest ≈ 8 levels of ortho and para-H₂O (over that of pure radiative pumping), providing a better fit to the observations; second, it also significantly affects some high-lying lines that, although radiatively pumped, are populated from the reservoir of H₂O in the low-lying levels. This combination of increased collisional excitation in the low-lying levels, coupled to the radiative pumping to upper levels, affects mainly the $8_{18} \rightarrow 7_{07}$ and $6_{15} \rightarrow 5_{24}$ transitions, which are strengthened by $\sim 40\%$ relative to models where collisional excitation is neglected.

Our best fit model for H₂O uses $\tau_{200} = 1-1.5$; a higher value (e.g. $\tau_{200} \approx 4$), still compatible with HCN, would produce too strong absorption in the H₂O lines at long wavelengths ($\geq 150 \mu\text{m}$, specifically in the $3_{03} \rightarrow 2_{12}$ transition in Fig. 4p). On the other hand, the covering factor for H₂O is slightly higher than for HCN. These points could indicate that the very excited HCN is more concentrated than H₂O (and mostly OH) toward the warmest region of C_{core} . Figures 3–19 indicate that the model

for C_{core} is satisfactory for a number of H₂O lines, and Fig. 5 shows that the model with $N_{\text{H}_2\text{O}} = 5 \times 10^{18} \text{ cm}^{-2}$ predicts absorption comparable to that observed in most of the marginally detected H₂O lines.

3.4.2. OH

The high-lying OH doublets in the $\Pi_{3/2}$ ladder at 65 and $53 \mu\text{m}$, and in the $\Pi_{1/2}$ ladder at 71 and $56 \mu\text{m}$, are compared in Fig. 6 (upper spectra) with the model for C_{core} (blue curves). In this model we have also adopted the same parameters as for H₂O, and the fit to OH shown in Fig. 6 is obtained with an OH abundance decreased by factor of 2.5 relative to that of H₂O. The OH 65 and $71 \mu\text{m}$ doublets are somewhat underestimated. The OH/H₂O ratio in C_{core} of NGC 4418, ~ 0.4 , is similar to that found in the nucleus of Arp 220. Like H₂O, the model for OH also favors $\tau_{200} \approx 1$ to avoid too strong absorption in the $163 \mu\text{m}$ doublet, and the covering factor for OH is higher than for HCN and H₂O (Table 2). Similar to Arp 220, all other OH lines have important contribution from a more extended region, and are discussed below in Sects. 3.5 and 3.6.

3.4.3. NH₃

The C_{core} model for NH₃, shown with red lines in Fig. 10, uses the same parameters as derived above for HCN: $n_{\text{H}_2} = 3 \times 10^6 \text{ cm}^{-3}$, $T_{\text{d}} = 150 \text{ K}$, and $T_{\text{g}} = 200$ and 250 K , but results for these two T_{g} values were found to be very similar. The NH₃ data are mostly compatible with $\tau_{200} \approx 1$. The derived column is $N_{\text{NH}_3} \approx 2.5 \times 10^{17} \text{ cm}^{-2}$, i.e. HCN/NH₃ ≈ 3 and $\chi_{\text{NH}_3} \approx 6 \times 10^{-7}$. In comparison with the model for Arp 220, the higher T_{d} in NGC 4418 translates into a higher excitation of non-metastable levels along a given K -ladder, and the higher T_{g} implies higher excitation across K -ladders. The former effect is responsible for the asymmetry between the 124.6 and $124.9 \mu\text{m}$ features in Fig. 10d, which is not fully accounted for by the model; nevertheless, the effect is sensitive to the overlap between the $K = 0$ and $K = 1$ lines. On the other hand, the model accounts for the absorption in the $(8, 6)_s \rightarrow (7, 6)_a$ line and, with the contribution of H₂O, for the feature at $63.47 \mu\text{m}$, though the marginal absorption in the $(8, 5)_s \rightarrow (7, 5)_a$ transition is not quite reproduced. As for Arp 220, the $(3, K)_a \rightarrow (2, K)_s$ feature (panel g) is not fully reproduced, suggesting a more extended, lower-excitation component for the low-lying lines.

3.4.4. H₂¹⁸O and ¹⁸OH

Relative to the main isotopologues, the H₂¹⁸O and ¹⁸OH lines in NGC 4418 are weaker than in Arp 220. We have modeled these lines in NGC 4418 with the same nuclear C_{core} model as for H₂O and OH, and modeled results are compared with observations in Figs. 7 and 8. For H₂¹⁸O, the model for the C_{core} component (red curves in Fig. 7) that reproduces the $3_{31} \rightarrow 2_{20}$ and $3_{21} \rightarrow 2_{12}$ lines uses a H₂O-to-H₂¹⁸O ratio of 500. While the model predictions are consistent with most observed H₂¹⁸O features, the relatively strong H₂¹⁸O $4_{23} \rightarrow 3_{12}$ line at $79.5 \mu\text{m}$ (Fig. 7d) is underestimated by the model. On the other hand, the ¹⁸OH lines are only marginally detected in the spectrum of NGC 4418. Our model (red lines in Fig. 8) also uses an OH-to-¹⁸OH ratio of 500, with the result that the undetected red $120.2 \mu\text{m}$ Λ -component and the ¹⁸OH $85 \mu\text{m}$ doublet are overpredicted. Still, the low SNR ¹⁸OH lines at 65 and $85 \mu\text{m}$ are affected by an uncertain baseline; owing to additional uncertainties in the OH column and

distribution, we estimate a lower limit for the OH-to- ^{18}O H ratio of 250. In summary, the ^{16}O -to- ^{18}O ratio in NGC 4418 is estimated to be $\gtrsim 250$, with a best fit overall value of ~ 500 .

3.5. The mid-excitation H_2O lines in NGC 4418: the warm component (C_{warm})

Figures 3 and 4 show that the model for C_{core} underestimates the absorption in some mid- and low-lying lines of H_2O ($3_{30} \rightarrow 2_{21}$, $3_{21} \rightarrow 2_{12}$, $3_{22} \rightarrow 2_{11}$, $2_{21} \rightarrow 1_{10}$, $4_{14} \rightarrow 3_{03}$, $3_{13} \rightarrow 2_{02}$, and $2_{12} \rightarrow 1_{01}$), and Fig. 1 indicates that the SED of the attenuated C_{core} cannot account for the bulk of the far-IR emission. Both points indicate the occurrence of another nuclear component that we denote as the warm component, C_{warm} .

The parameters for C_{warm} are more uncertain than those for C_{core} . Assuming that the continuum emission from C_{warm} is attenuated by the surrounding extended component (C_{extended}) described below, the dust temperature is ~ 85 – 110 K and $d \sim 30$ – 40 pc (Table 1). The model for the continuum and H_2O lines of C_{warm} is shown with light-blue curves in Figs. 1–4. The H_2O lines mentioned above can be reproduced with $N_{\text{H}_2\text{O}} \sim 5 \times 10^{16} \text{ cm}^{-2}$, much lower than toward C_{core} . With an estimated $\tau_{200} \approx 0.5$, the model for C_{warm} produces emission in some lines at $\lambda \gtrsim 130 \mu\text{m}$. The H_2O abundance is several $\times 10^{-7}$.

The model for C_{warm} is applied to OH in Fig. 6 (light-blue curves), with OH/ $\text{H}_2\text{O} = 0.4$. The main effect of C_{warm} is to increase the absorption in the 119 and $84 \mu\text{m}$ doublets, and to generate reemission in the $163 \mu\text{m}$ doublet. Nevertheless the joint contribution of the C_{core} and C_{warm} components predicts the $163 \mu\text{m}$ doublet in absorption, in contradiction to Fig. 6j, thus indicating the presence of a more extended component described below.

3.6. The low-lying lines in NGC 4418: the extended component (C_{extended})

Figure 11 compares the [O I] 63 and $145 \mu\text{m}$ lines and the 119, 79, 84 and $163 \mu\text{m}$ OH lines in NGC 4418 and Arp 220, emphasizing the different kinematics found in both sources. In Arp 220, the OH $163 \mu\text{m}$ doublet, and the emission features in the [O I] 63 and OH 79 μm transitions, are redshifted relative to the systemic velocity, and thus reveal outflowing gas though affected by foreground absorption. The broad [O I] $145 \mu\text{m}$ line supports this kinematic scenario. In NGC 4418, however, the line profiles are narrower than, and in some aspects opposite to those in Arp 220. The main spectral characteristics of these lines in NGC 4418, as discussed in Sect. 2.7, are: (i) the [O I] 63 μm absorption is redshifted by $\approx 110 \text{ km s}^{-1}$, and an emission feature is detected at blueshifted velocities; (ii) the absorption in the OH 119 and 79 μm lines is also redshifted by $\approx 100 \text{ km s}^{-1}$, with some indications of higher redshift in the 119 μm than in the 79 μm doublet (Fig. 14); (iii) a redshifted asymmetry is seen in the red Λ -component of the $84 \mu\text{m}$ doublet; (iv) the $163 \mu\text{m}$ doublet, with relatively low SNR, is detected in emission with one of the components apparently blueshifted with a velocity comparable to that of the [O I] 63 μm emission feature, though the other one peaks at central velocities. The lowest-lying H_2O line at $179.5 \mu\text{m}$ is also redshifted, but it is contaminated by CH^+ ($2 \rightarrow 1$).

On the other hand, the high-lying H_2O and OH lines in NGC 4418 do not show indications of any outflow, but peak at the rest-frame velocity as derived from for the optical absorption/emission lines. Only the ground-state [O I] and OH lines

are redshifted, together with some indications of a lower redshift in the excited OH $84 \mu\text{m}$ line. This indicates that this kinematic component is tracing a relatively low-excitation component around the galaxy nucleus. Near-IR observations (Evans et al. 2003) do not show evidence for a nearby “contaminating” companion where these lines could be formed (the closest galaxy, VV 655, is at ~ 25 kpc), but a linear, compact structure with fainter structures extending radially out to $\sim 1''$ (140 pc) in radius is apparent. This morphology may suggest that the redshifted spectral features are formed in (the inner region of) these extended streamers, thereby suggesting the possibility of an envelope inflowing onto the nucleus of NGC 4418.

We first constrain the column of the redshifted absorbing component in front of the nucleus by calculating the column of O I from the W_{eq} of the $63 \mu\text{m}$ absorption feature. Assuming that the line is optically thin at all velocities, that the shell covers the whole far-IR continuum source at $63 \mu\text{m}$ (43 Jy), and ignoring reemission in the line, we derive $N_{\text{O I}} = 5.3 \times 10^{18} \text{ cm}^{-2}$. This is a lower limit, as models described below indicate that there is significant reemission from the envelope (i.e. from C_{extended}) in both the $63 \mu\text{m}$ continuum and in the line; we estimate from the models a more accurate $N_{\text{O I}} = (1.4\text{--}1.8) \times 10^{19} \text{ cm}^{-2}$. Assuming a gas-phase O I abundance typical of translucent clouds ($\chi_{\text{O I}} = 2.5 \times 10^{-4}$ relative to H, Cartledge et al. 2001; Lis et al. 2001), $N_{\text{H}} \approx 6.5 \times 10^{22} \text{ cm}^{-2}$, or $A_{\text{v}} \sim 30$ mag. Since oxygen depletion may be enhanced for those columns (Bergin et al. 2000), the allowed range is $A_{\text{v}} \approx 30$ – 60 mag. This extinction is at least half of that required to account for the silicate absorption at $10 \mu\text{m}$.

One important parameter for the inflowing scenario is the amount of gas that is inflowing on the lateral and back sides of the nucleus. In order to constrain the geometry, calculations in spherical symmetry are performed and compared with data. The model for this extended component (C_{extended} in Tables 1 and 2) simulates a spherical envelope with inner and outer radii of $R_{\text{inner}} \approx 20$ and $R_{\text{outer}} \sim 100$ pc ($0.15''$ and $0.7''$) inflowing onto the warm nucleus. The value of R_{inner} is chosen to match the estimated outer radius of C_{warm} . The line profiles are best matched with a density profile that varies as $\sim r^{-2}$, with a highest value of $n_{\text{H}} = 2.5 \times 10^3 \text{ cm}^{-3}$ in the neighborhood of the nucleus. At R_{outer} , $n_{\text{H}} \approx 10^2 \text{ cm}^{-3}$, and thus the value for the outer radius is not critical. While the [O I] $63 \mu\text{m}$ absorption can be reproduced by either a turbulent shell inflowing with uniform $v = -110 \text{ km s}^{-1}$, or by assuming a radial velocity gradient across the envelope, the OH shifts in Fig. 14 suggest a progressive gas deceleration with decreasing distance to the galactic nucleus, with the thickest 119 μm line, tracing the outermost regions, showing the highest V_{shift} , and optically thinner (79 μm) or excited (84 μm) lines peaking closer to the rest velocity. We thus have empirically adopted a velocity field with -30 km s^{-1} at R_{inner} and $dv/dr = -2.1 \text{ km s}^{-1} \text{ pc}^{-1}$ (i.e. -200 km s^{-1} at R_{outer}), roughly simulating gas in nearly free-fall at the outermost radius, and subsequent deceleration due to radiation pressure (see Sect. 4.2.3) and/or interaction with orbiting gas, with gas approaching the systemic velocity in the neighborhood of the nucleus.

Our model for OH, shown in Fig. 11, includes both the nuclear component (the combined emission of the C_{core} and C_{warm} components is shown with blue lines) and the inflowing component (C_{extended} , green lines). An interesting feature of the line profiles is that, at central velocities where the excited lines show deep absorption (and the OH column densities are high), the absorption in the ground 119 and 79 μm lines is relatively weak. The model for the nucleus ($C_{\text{core}}+C_{\text{warm}}$) predicts too much absorption in these lines even adopting the high

density of $3 \times 10^6 \text{ cm}^{-3}$ and $T_g = 200 \text{ K}$ for C_{core} . Nevertheless, a reasonable match to the profiles involves partial cancellation between the absorption toward the continuum source and emission (through direct scattering at $119 \mu\text{m}$, and pumping through 53 and $35 \mu\text{m}$ for the $79 \mu\text{m}$ transition) from C_{extended} around the nucleus. This process also accounts for the emission in the $163 \mu\text{m}$ doublet, as every $163 \mu\text{m}$ photon should be accompanied, through downward cascade, by a $79 \mu\text{m}$ line photon. In the model, the $163 \mu\text{m}$ components are blueshifted by -45 km s^{-1} , but the observed shift is unclear as discussed in Sect. 2.7. On the other hand, the adopted velocity gradient predicts absorption at $\sim -50 \text{ km s}^{-1}$ in the $84 \mu\text{m}$ excited line, nearly matching the observed asymmetric $84 \mu\text{m}$ line shape. The model for OH is then consistent with an extended envelope and favors the scenario of an inflow extended on the lateral sides, though the lack of blueshifted emission in one of the Λ -components of the $163 \mu\text{m}$ doublet leaves the case inconclusive. The OH column across C_{extended} is $N_{\text{OH}} \approx 1.5 \times 10^{16} \text{ cm}^{-2}$, and $\chi_{\text{OH}} \sim (1.5-3) \times 10^{-7}$. From the absorption in the $\text{H}_2\text{O } 2_{12} \rightarrow 1_{01}$ line in Fig. 4q, which is contaminated by CH^+ , we estimate an uncertain $N_{\text{H}_2\text{O}} \sim 2 \times 10^{15} \text{ cm}^{-2}$.

The model for OH has been applied to O I. The absorption component of the $63 \mu\text{m}$ line is reproduced with an O I/OH abundance ratio of 10^3 , close to the value expected for translucent clouds. We first ignore the possible contribution by the nucleus to the emission feature of the [O I] $63 \mu\text{m}$ line. The resulting line shape is compared with the observed profile in Fig. 11a (green curve), and shows that (i) the velocity field and density profile adopted for OH roughly match the absorption in the [O I] $63 \mu\text{m}$ line, though the modeled absorption is somewhat overestimated at low velocities; (ii) in our spherically symmetric model, the emission feature is formed in the inflowing envelope through scattering of $63 \mu\text{m}$ photons, overestimating by 70% the flux of the observed spectral feature (325 Jy km s^{-1} between -200 and 0 km s^{-1}). Our model for O I thus supports an inflow with wide opening angle, but with the amount of gas inflowing on the lateral sides being lower than in front of it.

The above solution for the blueshifted emission in the [O I] $63 \mu\text{m}$ line, i.e. that the feature is formed in the inflowing envelope, is, however, not unique, because of the possible contribution by the nucleus to this feature. Indeed, the [O I] $145 \mu\text{m}$ line, though weak and too narrow as compared with the instrumental spectral resolution, is detected in the PACS spectrum (Fig. 11b), and the line should be formed in the nuclear region. Here we attempt to address the conditions under which the emission in the [O I] $63 \mu\text{m}$ line may be also formed in the nuclear region. We have then calculated the expected nuclear emission in the [O I] $63 \mu\text{m}$ line as a function of the assumed nuclear gas density. In all models, the nuclear O I column is fixed to match the observed [O I] $145 \mu\text{m}$ line. We have used a “mixed” approach as the continuum opacity at $145 \mu\text{m}$ is moderate and the inner regions of the nucleus can contribute to the [O I] $145 \mu\text{m}$ line. We have adopted the dust model for the C_{warm} component with $T_d = 110 \text{ K}$, and the gas at $T_g = 150 \text{ K}$. Collisional rates between O I and H_2 are taken from Jaquet et al. (1992). Results for the blueshifted (i.e. integrated between -200 and 0 km s^{-1}) emission are compared with the observed value in Fig. 20. At the relatively low density of 10^5 cm^{-3} , the excitation of the [O I] $63 \mu\text{m}$ line is below T_d , and the line is predicted in weak absorption. However, the absorption changes to emission for higher densities, and the blueshifted integrated flux attains a value comparable to the observed one at $n_{\text{H}_2} \approx 3 \times 10^6 \text{ cm}^{-3}$. Thus a significant contribution by the compact nucleus to the [O I] $63 \mu\text{m}$ emission feature is not ruled out from the point of view of the radiative

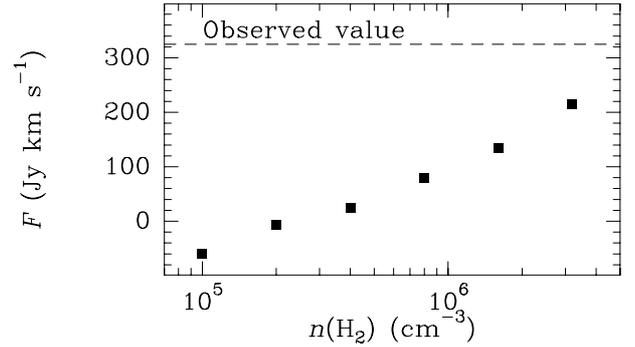


Fig. 20. Modeled [O I] $63 \mu\text{m}$ emission above the continuum, integrated over blueshifted velocities (i.e. between -200 and 0 km s^{-1} with respect to the systemic velocity), for the nucleus of NGC 4418 as a function of the H_2 density. The dashed line indicates the observed value.

transfer. For $n_{\text{H}_2} = 3 \times 10^6 \text{ cm}^{-3}$, the “mixed” O I column is $N_{\text{O}^0} \approx 1.5 \times 10^{20} \text{ cm}^{-2}$, and $\chi_{\text{O}^0} \sim 3 \times 10^{-5}$.

The case of the [O I] $63 \mu\text{m}$ emission appears then somewhat ambiguous on the basis of these radiative transfer models. Still, the OH models and the requirement of an extended region to account for the emission in the OH $163 \mu\text{m}$ doublet, favor C_{extended} as the main contributor to the [O I] $63 \mu\text{m}$ emission feature, but the relative contribution by the nucleus is hard to constrain. We further discuss this issue in Sect. 4.4.

3.7. The continuum of NGC 4418

Our continuum fit to NGC 4418, shown in Fig. 1a and with parameters listed in Table 1, is composed of: (i) a hot component (C_{hot} , yellow curve) with $T_d = 350 \text{ K}$ and an effective diameter of $d \approx 5 \text{ pc}$, attenuated by $A_V = 70 \text{ mag}$. It accounts for the mid-IR emission including the silicate $10 \mu\text{m}$ absorption; (ii) the nuclear core (C_{core} , blue curve) with $T_d = 150 \text{ K}$ and $d = 20 \text{ pc}$, attenuated by $A_V = 81 \text{ mag}$. It is required to explain the high-lying molecular absorption observed in H_2O , HCN, OH, and NH_3 ; (iii) the warm component (C_{warm} , light-blue curve) with $T_d = 110 \text{ K}$ and $d = 31 \text{ pc}$, attenuated by $A_V = 65 \text{ mag}$. The parameters of this component are somewhat uncertain and could include regions with lower $T_d \sim 85 \text{ K}$. C_{warm} mainly accounts for some mid-excitation lines of H_2O and OH; (iv) the extended component (C_{extended} , solid green curve) with non-uniform T_d and $d \approx 200 \text{ pc}$, which mainly accounts for the redshifted OH absorption and for the emission in the OH $163 \mu\text{m}$ doublet. The emission from the above components still underestimates the observed continuum at $\lambda \gtrsim 100 \mu\text{m}$, and therefore we have added a more extended, cold component with $d = 650 \text{ pc}$ and $T_d = 50-25 \text{ K}$ (dashed-green curve in Fig. 1a). This cold component, however, has no obvious molecular counterpart at far-IR wavelengths and is included in order to obtain a reasonable fit to the SED at long wavelengths, though the total emission (red curve in Fig. 1a) still underestimates the (sub)millimeter emission. Possible causes are the wavelength dependence of the dust absorption coefficient, and the uncertain dust opacity and size of the nuclear core at (sub)millimeter wavelengths.

The unattenuated luminosities of the hot, core, and warm components are $8.5 \times 10^{10} L_\odot$ (i.e. 85% of the bolometric luminosity), $\sim 7 \times 10^{10} L_\odot$, and $6 \times 10^{10} L_\odot$, respectively. The sum of the three exceeds the bolometric luminosity, implying that, unless there are important geometrical effects that make us underestimate the true galaxy luminosity, most emission of the core and warm components is not intrinsically generated, but largely

reemission due to heating from inside. Nevertheless, clear departures from spherical symmetry are inferred from our modeling, as e.g. the extinction affecting C_{hot} is much lower than the extinction through C_{core} , so the latter component can not be interpreted as a homogeneous shell surrounding C_{hot} .

4. Discussion

4.1. Model uncertainties

Our schematic models adopt uniform densities and uniform dust temperatures for the nuclear components, which is clearly a rough approach as it ignores their inner structures and clumpiness. The use of spherical symmetry is also certainly inaccurate, especially in NGC 4418 where a linear structure for the nuclear region is observed in the near-IR (Evans et al. 2003). Thus our models should be considered equivalent spherical/uniform approaches to complex structures.

Toward the nuclear region of Arp 220 and NGC 4418, our column density estimates are dust-limited, in the sense that the line absorption traces the outermost regions where $\tau_d < 1$. In this far-IR photosphere, we estimate that our derived columns per unit of τ_{50} are probably accurate to within 50% for a given T_d . Conversion to abundances is more uncertain. We have normalized the inferred column densities to a total H column of $N_{\text{H,norm}} = 4 \times 10^{23} \text{ cm}^{-2}$. However, the above H column depends on the gas-to-dust ratio as well as on the assumed properties of dust grains. Furthermore, the HCN absorption is observed at wavelengths longer than most H₂O and OH lines, and thus traces higher H columns than the latter species. The molecular abundances are thus reliable only to within a factor of 2–3. Nevertheless, abundance *ratios* between different molecular species are based on the same approach, and are therefore more accurate.

4.2. The nuclear regions of NGC 4418 and Arp 220

4.2.1. A hot core chemistry

The far-IR *Herschel*/PACS observations of NGC 4418 and Arp 220 reveal extreme excitation in the key molecular species H₂O, OH, HCN, and NH₃. The lines are observed mostly in absorption against the continuum, and our analysis indicates that very high column densities and abundances of these molecules surround (and are associated with) compact, far-IR thick, luminous continuum components.

One of the most intriguing results of our analysis is the high abundance derived for HCN, $(1-2) \times 10^{-6}$ in both Arp 220 and NGC 4418. At millimeter wavelengths, HCN has been found to be enhanced over HCO⁺ in ULIRGs (Graciá-Carpio et al. 2006) and in Seyferts over starbursts (Imanishi et al. 2007), and this has been proposed to be a diagnostic of AGN activity. Costagliola et al. (2011), however, argue that for high densities and columns HCO⁺ is expected to be stronger than HCN in XDRs (Meijerink et al. 2007). Models by Meijerink & Spaans (2005) predict HCN abundances and cumulative column densities in XDRs that fall by far too short to explain the values we derive in both NGC 4418 and Arp 220. Likewise, the peak HCN abundances predicted by Lepp & Dalgarno (1996) for XDRs, a few $\times 10^{-8}$, are about two orders of magnitude lower than the values we derive.

The high HCN abundances in both sources are very likely tracing a hot-core like chemistry, as has been proposed by previous authors, i.e. by Lahuis et al. (2007) from the HCN 14 μm

absorption in these and other (U)LIRGs, Martín et al. (2011) for Arp 220 based on multispecies observations at 1.3 mm, and Aalto et al. (2007a) and Costagliola & Aalto (2010) to explain the luminous HC₃N emission in NGC 4418. HCN is well known to be enhanced in Galactic hot cores, as in the Orion hot core where the abundance is $\sim 10^{-6}$ (Schilke et al. 1992), about two orders of magnitude higher than in cold molecular clouds. Time-dependent chemical models for hot cores by Rodgers & Charnley (2001) predict a linear increase of the HCN abundance with time for $T_g = 300$ K, attaining values of 10^{-5} relative to H₂ after $\sim 10^6$ yr of chemical evolution. The authors describe this model result as “pathological” as such high abundances are not found in Galactic hot cores, and suggest that these regions do not survive for more than a million years. However, extragalactic nuclear regions may survive long enough to develop such high HCN abundances.

The proposed evolved hot core chemistry finds support in the HCN/NH₃ ratio of 2–5 estimated in both Arp 220 and NGC 4418. After $\geq 10^6$ yr of chemical evolution, the models by Rodgers & Charnley (2001) predict that a similar value of the ratio can be reached provided that the gas temperature is high enough, though HCN is predicted to continue increasing with time. The ratio found by Rodgers & Charnley (2001) at such late stages of hot core evolution is independent of whether NH₃ was injected into the gas phase from mantles or formed directly in the gas phase.

The hot-core scenario is also quite consistent with the warm dust temperatures derived in the nuclear regions of NGC 4418 and Arp 220, and with the derived high H₂O abundances. In the Orion hot core, Melnick et al. (2010) derive H₂O abundances of $\sim 10^{-5}$ from *Herschel*/HIFI observations. Theoretically, an “undepleted chemistry” where grain mantles are evaporated is expected to increase the gas-phase H₂O abundance up to values $> 10^{-5}$ (e.g. Charnley 1997), i.e. orders of magnitude relative to the values inferred in cold molecular clouds and PDRs (Melnick & Bergin 2005), where H₂O ice is expected to be efficiently formed upon hydrogenation of atomic oxygen depleted on mantles in cold environments (Bergin et al. 2000; Hollenbach et al. 2009). If the gas attains sufficiently high temperatures ($T_g \sim 300$ K), H₂O will be further enhanced in the gas phase via neutral-neutral reactions (e.g. Elitzur & de Jong 1978).

The current models underpredict the low- J lines of HCN observed by Aalto et al. (2007a) in NGC 4418, who derived densities of $\sim 10^5 \text{ cm}^{-3}$; we derive much higher densities, $\sim 3 \times 10^6 \text{ cm}^{-3}$, for the high- J lines. Likewise, our models for the high- J lines in Arp 220 underpredict the $J = 6 \rightarrow 5$ measurement of Rangwala et al. (2011). It is plausible that these sets of lines probe different components, with the higher- J lines tracing very dense gas close to the regions of high far-IR emission with temperatures of $T_d > 100$ K, while the low- J lines trace a surrounding or interclump component with more moderate densities. No lines of HNC are found in the PACS spectra of NGC 4418 or Arp 220, while at millimeter wavelengths HNC is overluminous relative to HCN (Aalto et al. 2007b).

The high OH abundances in both NGC 4418 and Arp 220 do not easily fit into the hot core scenario. Observationally, OH observations of Orion BN/KL by Melnick et al. (1990) indicate that the emission/absorption is mostly produced by the shocked gas associated with the outflow, with little contribution, if any, by the hot core. Recently, Wampfler et al. (2011) derived a very low OH/H₂O $\sim 10^{-3}$ abundance ratio in the warm ($T > 100$ K), quiescent component of the Galactic high-mass star-forming region W3 IRS 5. Models by Charnley (1997) indeed predict a very low

OH/H₂O ratio in hot cores as most oxygen at high T is expected to be channelled into H₂O.

4.2.2. X- and cosmic rays

Another component, with chemistry dominated by photoprocesses and/or cosmic rays, is thus required to account for the OH enhancement in the nuclear region of both galaxies. Multitransition observations of OH in the Orion bar and chemical modeling by Goicoechea et al. (2011) reveal a dense/warm PDR component with an OH abundance of a few $\times 10^{-6}$. However, the OH enhancement is expected to be restricted to the external $A_V \lesssim 1$ layers where OH/H₂O > 1 due to H₂O photodissociation by the FUV field (Goicoechea et al. 2011). In NGC 4418 and Arp 220, we require widespread OH to account for the observations and, if PDRs alone are invoked, the surfaces of the nuclear regions in both sources (with typical sizes of 40 and 100 pc) would have to be covered with such high-density, low- A_V PDRs with a covering factor of ≥ 0.5 and, for typical individual PDR columns of $N_{\text{OH}} \sim \text{a few} \times 10^{15} \text{ cm}^{-2}$ (Goicoechea et al. 2011), ≥ 100 of such regions are needed along the line of sight. The impact of FUV photons on large amounts of gas can be enhanced under special geometries, as in the walls of cavities excavated by outflows (Bruderer et al. 2010); OH is boosted in outflows where H₂O is photodissociated by strong FUV fields (Melnick et al. 1990; Spinoglio et al. 2000). However, again a large number of overlapping outflows would be required across columns of several $\times 10^{23} \text{ cm}^{-2}$. Furthermore, the outflow signatures in Arp 220 are only observed in lines of moderate excitation, and NGC 4418 does not show any hint of outflowing gas, indicating that high-velocity (as compared with Galactic standards) outflows are not responsible for the observed chemistry. Nevertheless, the presence of Orion-like outflows with velocities of $\sim 30 \text{ km s}^{-1}$ is not ruled out.

A promising scenario to explain the high OH columns and abundances is through the effect of cosmic/X-rays, which penetrate in high- A_V regions much more deeply than UV photons. The OH/H₂O ratio as predicted by XDR and CR models of high density molecular regions is > 1 , and χ_{OH} easily exceeds 10^{-6} (Maloney et al. 1996; Meijerink et al. 2011). Large amounts of OH can be formed through dissociative recombination of H₃O⁺, which in turn is formed through the sequence $\text{O}^+ \rightarrow \text{OH}^+ \rightarrow \text{H}_2\text{O}^+ \rightarrow \text{H}_3\text{O}^+$ (Maloney et al. 1996); as we will report in a forthcoming paper, these molecular ions are indeed detected in absorption from excited levels in both sources. However, both NGC 4418 and Arp 220 have strong X-ray deficits relative to the FIR emission (Maiolino et al. 2003; Iwasawa et al. 2005). From the X-ray flux reported by Maiolino et al. (2003) from NGC 4418, $F_X(0.3\text{--}8 \text{ keV}) = 1.5 \text{ erg s}^{-1} \text{ cm}^{-2}$, and assuming a point-like X-ray source located at the center of our C_{core} component, the X-ray flux at the surface of C_{core} ($r \sim 10 \text{ pc}$) is $\sim 0.1 \text{ erg s}^{-1} \text{ cm}^{-2}$; a similar estimate for Arp 220 with the fluxes reported by Iwasawa et al. (2001) yields an X-ray (0.5–10 keV) flux at the surface of the western nucleus ($r \sim 50 \text{ pc}$) of $\sim 0.5 \text{ erg s}^{-1} \text{ cm}^{-2}$. Since the lines observed with PACS are formed around far-IR thick components with $N_{\text{H}} \geq 5 \times 10^{24} \text{ cm}^{-2}$, any putative strong and buried X-ray source would be severely extinguished, and the above distance-corrected estimates are probably lower limits due to foreground absorption but still relevant within a factor of 3. Conversion to ionization rates (ζ) and energy deposition rates per unit of hydrogen density (H_X/n) is very sensitive to the adopted X-ray spectrum (Wardle et al. 1999); adopting $\zeta (\text{s}^{-1}) \sim 2 \times 10^{-13} F_X (\text{erg s}^{-1} \text{ cm}^{-2})$, we infer $\zeta \sim (0.2\text{--}1) \times 10^{-13} \text{ s}^{-1}$ and $H_X/n \lesssim (1\text{--}5) \times 10^{-30} \text{ erg cm}^3 \text{ s}^{-1}$

(Maloney et al. 1996) for NGC 4418-Arp 220 in the far-IR nuclear photosphere traced by the OH. It is unclear if such low energy deposition rates per unit density can produce the high nuclear OH abundance we measure at least in NGC 4418, where very high densities are found. Nevertheless, cosmic rays are an alternative, and both X- and cosmic rays could efficiently generate OH from a high reservoir of H₂O that is formed by other means (i.e. by a hot core chemistry or by low-velocity outflows), through photodissociation of H₂O by internally generated UV photons (Gredel et al. 1989; Wardle et al. 1999) and/or reactions of H₂O with He⁺, H⁺, H₂⁺, and H₃⁺ to form OH directly or via the H₂O⁺ and H₃O⁺ intermediates; this high H₂O reservoir is evident in both sources. Detailed chemical modeling is required to differentiate between these, and other alternatives; while H₂O may be expected to be abundant in regions where HCN-NH₃ or OH are enhanced, it remains to be determined whether the HCN-NH₃ and the OH can be co-spatial.

4.2.3. Sources of luminosity

The presence of high columns of HCN and H₂O and the implied hot core chemistry in the nuclear regions neither supports nor rules out the presence of a deeply buried AGN. It could simply indicate that, regardless of the nature of the intrinsic luminosity source(s), frequency degradation in a very thick medium (as UV radiation is absorbed by dust and re-emitted at longer wavelengths by sampling progressively colder media), makes far-IR photons more relevant for the chemistry of large fractions of the nuclear gas (through dust heating and mantle evaporation) than the quickly absorbed UV photons.

Taking the Galactic Orion hot core as a template, its size ($\sim 10''$ diameter, or 0.02 pc at 414 pc; e.g. Wilson et al. 2000) is ~ 900 and ≥ 4000 times smaller (and the square of these numbers in surface) than those estimated for the C_{core} and C_{west} components of NGC 4418 and Arp 220, respectively. If the HCN absorption is interpreted in terms of hot cores around young stars, then $\sim 8 \times 10^4$ and $\sim 1.5 \times 10^7$ cores are inferred, respectively. Likewise, if a typical hot core harbors a luminous star with $10^5 L_{\odot}$, $\sim 7 \times 10^5$ and $\sim 7 \times 10^6$ young stars are inferred, respectively. This interpretation, however, has the drawback that Galactic hot cores are short lived, with a time scale of order 10^5 yr (Wilner et al. 2001). Even if the high pressure in the nuclear regions (Spoon et al. 2005) allows the hot cores to survive longer, a synchronized birth of $\sim 10^7$ hot cores in $< 1 \text{ Myr}$ over spatial scales of $\geq 80 \text{ pc}$, involving a propagation velocity of stellar formation of $> 100 \text{ km s}^{-1}$, seems unlikely. The observed absorption is rather interpreted in terms of large hot-core like structures (disk/torus/envelope) not necessarily associated with the very first stages of star formation.

The inferred hot core chemistry, complemented by the strong effects of X- and/or cosmic rays, is found to be physically associated with warm and luminous sources of far-IR emission. The surface brightnesses of the nuclear regions in both sources are very high, $\sim 7 \times 10^{13} L_{\odot}/\text{kpc}^2$ over 20 pc for the C_{core} component of NGC 4418, and $(0.9\text{--}4) \times 10^{13} L_{\odot}/\text{kpc}^2$ over 150–80 pc for the western nucleus of Arp 220. In the latter source, these are lower limits if the dust is heated from inside (Downes & Eckart 2007). Sa8 indicates that the luminosity from the Arp 220 western nucleus could be generated by 200–1000 super-star clusters. An important contribution from star formation to the luminosity of the western nucleus is indeed evident (e.g., Smith et al. 1998; Lonsdale et al. 2006), and the apparent lack of strong X-ray emission from X-ray binaries associated with star

formation (Lonsdale et al. 2006) can be interpreted in terms of extreme absorption column densities (Sa08, this work).

On the other hand, the broad 1.6 GHz OH megamaser emission terminal velocity of 800 km s^{-1} in Arp 220 (Baan et al. 1989), comparable to those of OH in the far-IR absorption lines of AGN driven ULIRGs (Fischer et al. 2010; Sturm et al. 2011), is much higher than the OH velocities observed in the far-IR spectrum of Arp 220. We interpret this as evidence for both far-IR extinction of the high velocity gas accelerated in the innermost nuclear region and deceleration of the outflowing gas with increasing involved columns. A very compact source for the outflowing gas would also support the presence of an energetically significant, strongly buried AGN that would also explain the somewhat different distributions traced by the compact centimeter-wave sources and the submillimeter continuum emission (Sa08). In NGC 4418, the extreme HCN and H₂O excitation on a scale of 20 pc in diameter, the large fraction of luminosity coming from such a compact region, and the indications of internal heating, favor the scenario of a far-IR thick disk/torus/envelope surrounding a nascent AGN, as has been proposed in previous works (e.g. Spoon et al. 2001), or a hyper-star cluster ~ 70 times more luminous than the super-star cluster in NGC 5253 (Turner et al. 2000).

In NGC 4418, the outward acceleration due to radiation pressure can be described by $a_{\text{rad}} \sim \kappa \sigma T_{\text{d}}^4 / c \sim (2-5) \times 10^{-6} \text{ cm s}^{-2}$, where $\kappa \sim 2-5 \text{ cm}^2 \text{ g}^{-1}$ is the Rosseland mean opacity at 100–150 K (Thompson et al. 2005) and σ is the Stefan-Boltzmann constant. We find that a_{rad} is similar to the gravitational acceleration, $a_{\text{grav}} = GM/R^2 \sim (2.5-5) \times 10^{-6} \text{ cm s}^{-2}$, where $M = (1.6-3.2) \times 10^7 M_{\odot}$ (for $\tau_{200} \sim 1-2$) and $R = 10 \text{ pc}$ have been estimated (Table 1). If the stellar mass is not much higher than the gas mass in the C_{core} component, the above comparison suggests that radiation pressure plays an important role in supporting the nuclear structure against self-gravity in an Eddington-like limit (Scoville 2004). In Arp 220 (C_{west}) radiation pressure appears less important due to the higher M/R^2 and lower⁴ T_{d} . Nevertheless, the disk in the western nucleus may be inclined such that our view of the warmer dust is obscured in the far-IR and we have a “rotationally-supported” edge-on view of the structure.

4.3. The extended component of Arp 220

The extended and halo components (C_{extended} and C_{halo}) in Arp 220 reveal a chemistry very different from that found in the nuclear region. The H₂O abundance drops to the relatively low value of $\sim 5 \times 10^{-8}$, typical of Galactic PDR regions, and the OH/H₂O ratio reverses the nuclear value becoming >1 , as in Galactic translucent clouds (e.g. Neufeld et al. 2002). Our estimated OH abundances of several $\times 10^{-7}$ are in general agreement with those derived by Polehampton et al. (2005) in the intervening translucent clouds toward Sgr B2. On the other hand, the outflow signatures observed in the OH 163 and 79 μm doublet, in the [O I] 63 and 145 μm lines (Fig. 11), and in the H₂O $3_{03} \rightarrow 2_{12}$ line (Fig. 4p), appear to indicate that the outflow is spatially extended on the back side of the nuclei.

The extended component of Arp 220 resembles the translucent Galactic medium, though with a higher ionization rate as

⁴ Vertical radiation pressure support in optically thick nuclear disks imply $\kappa T_{\text{eff}}^4 \propto \Sigma_{\text{g}}$ (e.g. Thompson et al. 2005), where T_{eff} is the effective dust temperature and Σ_{g} is the gas column. Comparison of NGC 4418 (C_{core}) and Arp 220 (C_{west}) indicates, however, lower T_{eff} and higher Σ_{g} in Arp 220.

derived from the absorption in lines of molecular ions, as we will report in a forthcoming paper.

4.4. Inflowing gas in NGC 4418?

The intriguing redshifted absorption in the ground-state lines of OH and O I, and the blueshifted emission in the [O I] 63 μm line, caused us to consider in Sect. 3.6 the possibility that an extended envelope around the nucleus of NGC 4418 is inflowing onto the nuclear region, thus feeding the nucleus and providing an external ram pressure that may further confine the nuclear gas. Krug et al. (2010) have reported the detection of inflows in Seyferts based on absorption measurements of the Na I doublet at optical wavelengths.

The morphology of the region as seen at near-IR wavelengths (Evans et al. 2003) and the absorption depths indeed suggest that the redshifted absorbing component is more than a single cloud in the galaxy disk with an anomalous velocity; the redshifted absorption affects the whole column of gas external to the nuclear region ($\sim 10^{23} \text{ cm}^{-2}$), as otherwise the ground-state OH absorption at the systemic velocity would be deeper than observed. Thus the OH and O I absorptions suggest bulk inward gas motions.

If spherical symmetry is assumed for this component, a mass inflow rate of $12 M_{\odot} \text{ yr}^{-1}$ is obtained at the surface of the nucleus, based on the model shown in Fig. 11. Spherical symmetry is consistent with the OH line profiles, in particular with the emission in the OH 163 μm doublet. However, the spherical approach overpredicts the [O I] 63 μm blueshifted emission (Fig. 11a). Furthermore, pure radiative transfer cannot rule out that a significant fraction of the [O I] 63 μm emission feature is formed in the nucleus, rather than in the envelope, if the high density component (several $\times 10^6 \text{ cm}^{-3}$, as derived from OH, H₂O, and HCN) is sufficiently rich in atomic oxygen (a few $\times 10^{-5}$). Observational surveys of the [O I] 63 μm line in Galactic hot cores may help further evaluate the latter possibility, but pure hot core chemistry predicts O I to have an abundance of only $\lesssim 10^{-6}$ (Charnley 1997). Guided by these models, we do not expect much contribution from dense hot cores to the [O I] 63 μm emission feature. However, the high-lying OH lines are tracing a region where photodissociation of H₂O is probably taking place (Sect. 4.2.2), so OH photodissociation could produce significant columns of dense O I. Still, the C-shock models by Wardle et al. (1999) with enhanced H₂O photodissociation due to X- or cosmic rays produce little O I, with OH/OI > 100 , but models for XDRs and CRs by Meijerink & Spaans (2005) and Meijerink et al. (2011) predict large amounts of oxygen in atomic form, though they use densities significantly lower than $3 \times 10^6 \text{ cm}^{-3}$.

In summary, our observations and analysis favor an inflow in NGC 4418, though the geometry and inflow rate of the inflowing gas are rather uncertain. If the gas were inflowing only from the front side of the nucleus with an opening angle of, say, 90° , the mass inflow rate would be of only $\approx 2 M_{\odot} \text{ yr}^{-1}$. Kawara et al. (1990) first suggested a possible inflow in NGC 4418 based on the narrow CO $J = 1-0$ line. The interaction with the nearby galaxy VV 655 could have triggered the inflow via a close (perigalactic), non-merging encounter $\sim 10^8 \text{ yr}$ ago for an average velocity difference of $\sim 200 \text{ km s}^{-1}$ in the plane of the sky, and models (Noguchi 1988; Iono et al. 2004) predict that the inflow triggered by interacting galaxies may last that long. Alternatively, a non-axisymmetric gravitational potential as in barred galaxies can fuel the nuclear region with large amounts of gas (Friedli & Benz 1993), which is supported by the peculiar morphology of NGC 4418.

4.5. Evolutionary effects

In spite of the very different global parameters (mass, luminosity, size, and merger versus non-merger class) of Arp 220 and NGC 4418, their nuclear regions share common properties. They contain warm dust, very excited molecular absorption, and high surface column densities of H₂O, OH, HCN, and NH₃. There are, however, significant differences in the properties revealed by their far-infrared spectra that probably stem from and further probe their individual evolutionary histories. The smaller, less massive, and less luminous NGC 4418 shows warmer dust and higher molecular excitation than Arp 220. Perhaps the most suggestive spectroscopic differences between the two sources are their inferred kinematics and ¹⁶O to ¹⁸O ratios: while NGC 4418 appears to have a ratio similar (to within a factor of 2) to that seen in the local solar neighborhood, the ratio in Arp 220 is significantly lower.

The outflow signatures in Arp 220, which range from 800 km s⁻¹ in its OH megamaser radio emission to 100 km s⁻¹ in submillimeter transitions of HCO⁺ and CO and up to 500 km s⁻¹ in some moderate excitation submillimeter and far-IR emission lines, suggest that injection of enriched gas from current and previous stellar processing has occurred. On the other hand, mechanical feedback has not yet occurred in NGC 4418, which may still be in a stage of inflow. Analysis of the H₂¹⁸O and the ¹⁸OH lines indicate ¹⁶O-to-¹⁸O ratios of 70–130 in Arp 220, reminiscent of the low ratio of ~40 derived for Mrk 231 (Fischer et al. 2010). The strong absorption in the red Λ -component of the ground-state ¹⁸OH 120 μ m doublet (Fig. 8c) indicates that the ¹⁸O enhancement is not restricted to the nuclear region, but also applies to the C_{extended} and C_{halo} components. At millimeter wavelengths, Martín et al. (2011) derive a ¹⁶O-to-¹⁸O ratio of >80 in Arp 220, while Harrison et al. (1999) estimated a ratio of ~150 in NGC 253. In NGC 4418, however, we find that the ¹⁶O-to-¹⁸O ratio is ≥ 250 , with a best fit value of ~500. While ¹⁶O is a primary product of stellar nucleosynthesis, ¹⁸O is a secondary one, and this ratio decreases with increasing star forming generations (Prantzos et al. 1996). Since galactic outflows are dominated by entrained ISM gas (Veilleux et al. 2005), the low ratios found in Arp 220 and Mrk 231 probably trace stellar processing throughout the merger lifetime. The apparent ISM inflow, lack of outflowing gas, and higher ¹⁶O-to-¹⁸O ratios in NGC 4418 appear to indicate an earlier evolutionary phase in the lifetime of the central AGN or nuclear starburst.

We tentatively suggest that the nuclei of Arp 220 and NGC 4418 are in an earlier evolutionary phase than the QSO driven ULIRG Mrk 231 (e.g. Veilleux et al. 2009). In this source, high velocity (~1000 km s⁻¹) feedback (Fischer et al. 2010; Sturm et al. 2011; Rupke & Veilleux 2011) in the form of a massive molecular/atomic outflow has more strongly disrupted its nuclear interstellar medium, as evidenced by the lower dust opacity of its warm component (González-Alfonso et al. 2010) compared with the nuclear regions of NGC 4418 and Arp 220. The lack of measurable HCN emission/absorption in its *Herschel*/SPIRE spectrum (van der Werf et al. 2010), suggests that exposure to UV and X-ray emission from its AGN appears to have at least partially shut down the hot core nitrogen chemistry⁵. Further, analysis of *Herschel*/SPIRE observations of H₂O emission in Mrk 231 (González-Alfonso et al. 2010) suggest an H₂O abundance of ~10⁻⁶, significantly lower than

in NGC 4418 and Arp 220, but observations of the same lines would help verify this issue. Lastly, the stronger stellar processing suggested by the increased enhancement of ¹⁸OH in Mrk 231 may indicate an older age of its merger induced star-formation than in Arp 220. This evolutionary scenario is consistent with the fact that in the mid-IR Mrk 231 looks AGN-like, while Arp 220 and NGC 4418 are still dominated by deep silicate absorption indicative of a buried, earlier evolutionary stage (Spoon et al. 2007).

5. Conclusions

The salient observational results presented here on NGC 4418 and Arp 220 are:

- Full range PACS spectroscopy of NGC 4418 and Arp 220 reveals high excitation in H₂O OH, HCN, and NH₃. In NGC 4418, absorption lines were detected with $E_{\text{lower}} > 800$ K (H₂O), 600 K (OH), 1075 K (HCN), and 600 K (NH₃), while in Arp 220 the excitation is somewhat lower with $E_{\text{lower}} > 600$ K (H₂O), 600 K (OH), 650 K (HCN), and 400 K (NH₃).
- More specifically, NGC 4418 shows 38 H₂O lines in absorption, and with marginal detections of even higher-lying lines, while Arp 220 shows absorption in 28 H₂O lines. All strong OH lines within the PACS domain are detected in both sources. In NGC 4418, at least 6 HCN rotational lines, from $J = 18 \rightarrow 17$ to $J = 23 \rightarrow 22$ with E_{lower} from 650 to 1075 K are detected in absorption, while the $J = 18 \rightarrow 17$ and possibly the $J = 21 \rightarrow 20$ lines are detected in Arp 220. Rotational NH₃ lines arising from E_{lower} up to ~600 K are detected in NGC 4418, while Arp 220 shows NH₃ lines up to ~400 K. Molecular absorption equivalent widths from high-lying levels are higher in NGC 4418 than in Arp 220.
- Up to 10 lines of H₂¹⁸O and 3 ¹⁸OH Λ -doublets are detected in Arp 220, while 6 H₂¹⁸O lines are detected in NGC 4418, where only a marginal detection of ¹⁸OH is found. The lines of the rare isotopologues are thus significantly stronger in Arp 220 than in NGC 4418.
- Lines with moderate excitation in Arp 220 show indications of outflowing gas, specifically in the redshifted emission features observed in lines of H₂O, OH, and O I. The absorption in more excited molecular lines peak at central velocities relative to our adopted redshift of 0.0181, though a contribution to the absorption by outflowing gas with velocities up to ~150 km s⁻¹ is not ruled out. In NGC 4418, however, the molecular lines do not show any indication of outflowing gas, and the absorption in the low-lying OH doublets as well as in the [O I] 63 μ m line are redshifted.

We have analyzed the observed absorption-dominated line profiles together with the far-IR continuum, using multicomponent radiative transfer modeling with a minimum number of parameterized components. The conclusions stemming from the analysis are:

- Extremely high H₂O column densities per unit of continuum optical depth at 50 μ m (τ_{50}), $\geq 3 \times 10^{18}$ cm⁻², and OH/H₂O and HCN/H₂O ratios of ≈ 0.5 and 0.1–0.3, respectively, are derived in the nuclear region of NGC 4418, along with dust temperatures ~150 K in the very inner nuclear core. In the nuclear region of Arp 220, T_d is in the range 90–130 K, implying H₂O columns of (6–0.8) $\times 10^{18}$ cm⁻² per τ_{50} and OH/H₂O and HCN/H₂O ratios similar to those of NGC 4418.

⁵ But not completely: during the final revision of this manuscript, Aalto et al. (2012) reported the detection of bright HC₃N (10–9) in the nuclear region of Mrk 231.

The HCN/NH₃ ratios are 2–5 in both sources. The continuum emission in these nuclear regions is optically thick at far-IR wavelengths in both galaxies.

- The nuclear molecular abundances relative to H are estimated to be high, with $\chi_{\text{H}_2\text{O}} \sim 10^{-5}$ in NGC 4418 and $(0.2\text{--}1.5) \times 10^{-5}$ in Arp 220.
- The absorption by the ¹⁸O isotopologues indicate a strong enhancement of ¹⁸O in Arp 220, with a ¹⁶O-to-¹⁸O ratio of 70–130, while the ratio in NGC 4418 is significantly higher, ≥ 250 with a best fit value of ~ 500 . The apparent ¹⁸O enhancement in Arp 220 probably traces stellar processing throughout the merger lifetime.
- We also require an extended component to produce the absorption in the low-lying lines of OH and H₂O; the fractional H₂O abundance in Arp 220 drops in this region to $\sim 5 \times 10^{-8}$ and the OH/H₂O is reversed relative to the nuclear region to 2.5–10. In the envelope of NGC 4418, we find $\chi_{\text{OH}} = \text{a few} \times 10^{-7}$.
- The extreme H₂O, HCN, and NH₃ columns and abundances in the nuclear region of both galaxies, together with the high dust temperatures, are interpreted in terms of a hot core chemistry, where grain mantles are evaporated. The high OH columns and abundances require in addition photoprocesses due to X-rays and/or enhancement by high cosmic ray fluxes. H₂O and OH may also be boosted in low-velocity shocks with enhanced H₂O photodissociation.
- Very thick ($N_{\text{H}} \geq 10^{25} \text{ cm}^{-2}$) nuclear media are responsible for the frequency degradation of the intrinsic luminosity in both sources, as high energy photons are absorbed and re-emitted at far-IR wavelengths sampling progressively colder media. Such conditions, and not necessarily a starburst-dominated luminosity, may also be responsible for the hot core chemistry in the nuclear regions. The high surface brightnesses, $\approx 6 \times 10^{13}$ and $(0.9\text{--}4) \times 10^{13} L_{\odot}/\text{kpc}^2$ on spatial scales of ~ 20 and $150\text{--}80$ pc in NGC 4418 and Arp 220, respectively, indicate either strongly buried AGNs or hyper star clusters. In NGC 4418, radiation pressure is probably responsible for the support of the nuclear structure against self-gravity.
- Both the outflowing gas and the low ¹⁶O-to-¹⁸O ratio in Arp 220 suggest a stage more evolved than in NGC 4418, but less evolved than the QSO driven ULIRG Mrk 231.
- In NGC 4418, the redshifted absorption observed in the low-lying OH and [O I] lines is best explained in terms of an envelope inflowing onto the nuclear region, but the geometry of this inflow is rather uncertain; we estimate the mass inflow rate to be $\lesssim 12 M_{\odot} \text{ yr}^{-1}$.

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