Herschel: observations of water vapour in Markarian 231


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ABSTRACT

The Ultra luminous infrared galaxy (ULIRG) Mrk 231 reveals up to seven rotational lines of water (H$_2$O) in emission, including a very high-lying ($E_{\text{upper}} = 640$ K) line detected at a 4$\sigma$ level, within the Herschel/SPIRE wavelength range (190 $\mu$m $< \lambda < 640$), whereas PACS observations show one H$_2$O line at 78 $\mu$m in absorption, as found for other H$_2$O lines previously detected by ISO. The absorption/emission dichotomy is caused by the pumping of the rotational levels by far-infrared radiation emitted by dust, and subsequent relaxation through lines at longer wavelengths, which allows us to estimate both the column density of H$_2$O and the general characteristics of the underlying far-infrared continuum source. Radiative transfer models including excitation through both absorption of far-infrared radiation emitted by dust and collisions are used to calculate the equilibrium level populations of H$_2$O and the corresponding line fluxes. The highest-lying H$_2$O lines detected in emission, with levels at 300–640 K above the ground state, indicate that the source of far-infrared radiation responsible for the pumping is compact (radius = 110–180 pc) and warm ($T_{\text{gas}} = 85–95$ K), accounting for at least 45% of the bolometric luminosity. The high column density, $N$(H$_2$O) $\sim 5 \times 10^{17}$ cm$^{-2}$, found in this nuclear component, is most probably the consequence of shocked/cosmic rays, an XDR chemistry, and/or an “undepleted chemistry” where grain mantles are evaporated. A more extended region, presumably the inner region of the 1-kpc disk observed in other molecular species, could contribute to the flux observed in low-lying H$_2$O lines through dense hot cores, and/or shocks. The H$_2$O 78 $\mu$m line observed with PACS shows hints of a blue-shifted wing seen in absorption, possibly indicating the occurrence of H$_2$O in the prominent outflow detected in OH (Fischer et al. 2010, A&A, 518, L41). Additional PACS/HIFI observations of H$_2$O lines are required to constrain the kinematics of the nuclear component, as well as the distribution of H$_2$O relative to the warm dust.

Key words. ISM: molecules – galaxies: ISM – galaxies: individual: Mrk 231 – line: formation – infrared: ISM – submillimeter: galaxies

1. Introduction

One key question in the study of composite infrared (IR) merging galaxies and quasi-stellar objects (QSOs) is what fraction of their luminosity is generated in the nuclear region ($<$200 pc) associated with the active galactic nucleus (AGN) and a possible extreme nuclear starburst, and what fraction arises from a more extended kpc-scale starburst (e.g. Armus et al. 2007; Veilleux et al. 2009). The ULIRG Markarian 231 (Mrk 231) is the most luminous ($L \sim 4 \times 10^{12} L_\odot$) galaxy in the local Universe ($z < 0.1$), and thus provides a unique template for such studies. Since the bulk of the luminosity in ULIRGs arises at far-IR wavelengths, where sub-arc-second resolution observations are not available, an alternative technique is required to constrain the compactness of the far-IR emission and its physical origin.

In a previous work based on observations with the ISO, González-Alfonso et al. (2008, hereafter G-A08) have argued that the observation of molecular species such as OH and H$_2$O at far-IR wavelengths is ideal for such a purpose, because their high-lying rotational levels are pumped through absorption of far-IR radiation and the observable excitation is then sensitive to the far-IR radiation density that in turn depends on the compactness of the far-IR continuum source. In addition, these molecular observations shed light on the dominant chemistry in those nuclear regions. G-A08 reported the ISO detection of 3 high-lying H$_2$O lines, relevant upper limits over the entire ISO spectrum, and also high-lying OH lines, indicating the occurrence of a compact-luminous far-IR component.

With their high sensitivity, spectral resolution, and wavelength coverage, the Herschel (Pilbratt et al. 2010) instruments are ideal for extending our previous study to additional key lines in the far-IR/submillimeter. As part of the HerCULES Key Programme (see van der Werf et al. 2010, hereafter vdW10), we report in this Letter the Herschel SPIRE/PACS (Griffin et al. 2010; Poglitsch et al. 2010) detection and first analysis of several H$_2$O lines in Mrk 231, which supports the conclusions of G-A08 and gives additional clues to the origin of H$_2$O in this ULIRG. We adopt a distance to Mrk 231 of 192 Mpc ($H_0 = 70$ km s$^{-1}$ Mpc$^{-1}$, $\Omega_k = 0.73$, and $z = 0.04217$).

2. Observations

The SPIRE FTS observations of Mrk 231 (vdW10) were conducted on December 9th, 2009. The PACS observation of one H$_2$O line was conducted on November 8th, 2009, as part of the SHINING key programme, and kindly provided for the present study. Details on data reduction, calibration, and line extraction
are given in vdW10 and Swinyard et al. (2010). Excerpts of the spectrum around the H$_2$O lines are displayed in Fig. 1, and an energy level diagram indicating the lines detected with SPIRE, the one detected with PACS, and those detected with ISO is shown in Fig. 2. Table 1 lists the line fluxes. Figure 1 also shows the results of our reference model, discussed below.

H$_2^18$O could be marginally detected at 250.0 $\mu$m (2$_{20}$$\rightarrow$2$_{11}$) (see vdW10); however, this identification should be confirmed as the feature is shifted by 150 km s$^{-1}$ from the nominal line wavelength. Confirmation of H$_2^18$O would be important as its presence would support the strong enhancement of $^{18}$O in Mrk 231 derived from $^{18}$OH observations (Fischer et al. 2010, hereafter F10). A number of the H$_2$O lines in Fig. 1 are blended with the C$^{18}$O lines 9$\rightarrow$8 (303.57 $\mu$m), 10$\rightarrow$9 (273.24 $\mu$m), and 11$\rightarrow$10 (248.43 $\mu$m). Contamination by C$^{18}$O is minimal, however, as the lower-lying 6$\rightarrow$5, 7$\rightarrow$6, and 8$\rightarrow$7 lines are not detected. PACS observations show a broad absorption feature at 121.7 $\mu$m, nearly coincident with the H$_2$O $\nu_2$ 12$\rightarrow$11 line (F10). However, this feature is probably contaminated by HF (2$\rightarrow$1) at the same wavelength, as the 1$\rightarrow$0 line is detected with SPIRE (vdW10); HF has been previously detected towards the Galactic star forming region Sgr B2 (Neufeld et al. 1997). Therefore the 121.7 $\mu$m feature is not used for the H$_2$O analysis below.

Of particular interest is the detection of the very high-lying 5$_{23}$$\rightarrow$5$_{14}$ H$_2$O line at a 4$\sigma$ level, which we have verified by reprocessing the data with no correction applied for the instrument spectral efficiency and by comparing these data with reduced observations of the dark sky over the same spectral range. The ground state lines (p-H$_2$O 1$_{11}$$\rightarrow$0$_{00}$ in Fig. 1 and o-H$_2$O 1$_{10}$$\rightarrow$0$_{01}$) are not detected. The lines detected with SPIRE are all in emission and peak at central velocities, in contrast to the low-lying OH lines that show P-Cygni profiles characteristic of an extreme molecular outflow (F10). The red horizontal lines indicate the FWHM of an unresolved line, and show that the H$_2$O lines detected with SPIRE are barely resolved. The o-H$_2$O 4$_{23}$$\rightarrow$3$_{12}$ line detected with the higher spectral resolution of PACS is in absorption and well resolved, showing a central main body and, apparently, a relatively weak blueshifted wing extending up to $\sim$800 km s$^{-1}$ and possible low level

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**Table 1. Observed and modeled line fluxes.**

<table>
<thead>
<tr>
<th>Line</th>
<th>Flux$^b$ (Jy km s$^{-1}$)</th>
<th>Model Flux$^b$ (Jy km s$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>p-H$<em>2$O 1$</em>{11}$$\rightarrow$0$_{00}$</td>
<td>269.27 &lt;300</td>
<td>177</td>
</tr>
<tr>
<td>o-H$<em>2$O 1$</em>{10}$$\rightarrow$0$_{01}$</td>
<td>538.29 &lt;400</td>
<td>146</td>
</tr>
<tr>
<td>p-H$<em>2$O 2$</em>{22}$$\rightarrow$1$_{11}$</td>
<td>303.46 718 (110)</td>
<td>660</td>
</tr>
<tr>
<td>p-H$<em>2$O 2$</em>{21}$$\rightarrow$1$_{10}$</td>
<td>398.64 415 (43)</td>
<td>365</td>
</tr>
<tr>
<td>p-H$<em>2$O 2$</em>{20}$$\rightarrow$1$_{10}$</td>
<td>243.97 342 (92)</td>
<td>372</td>
</tr>
<tr>
<td>o-H$<em>2$O 3$</em>{12}$$\rightarrow$2$_{03}$</td>
<td>273.19 400 (130)</td>
<td>438</td>
</tr>
<tr>
<td>o-H$<em>2$O 3$</em>{11}$$\rightarrow$2$_{02}$</td>
<td>257.79 631 (47)</td>
<td>657</td>
</tr>
<tr>
<td>o-H$<em>2$O 4$</em>{22}$$\rightarrow$3$_{13}$</td>
<td>248.25 361 (38)</td>
<td>381</td>
</tr>
<tr>
<td>o-H$<em>2$O 4$</em>{21}$$\rightarrow$3$_{12}$</td>
<td>212.53 287 (83)</td>
<td>269</td>
</tr>
<tr>
<td>o-H$<em>2$O 4$</em>{20}$$\rightarrow$3$_{11}$</td>
<td>78.74 &lt;910$^{-1}$ (60)</td>
<td>-664</td>
</tr>
</tbody>
</table>

**Notes:**

(a) Numbers in parentheses indicate the estimated uncertainties;

(b) includes the absorption in the high-velocity blue-shifted wing, which accounts for $\sim$220 Jy km s$^{-1}$.

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**Fig. 2.** Energy level diagram for H$_2$O, showing the detected/undetected (blue arrows/lines) lines with SPIRE, the line detected with PACS (green) and those detected by ISO (light blue). Dashed red arrows indicate the main pumping paths for the high-lying lines observed with SPIRE. Upward (downward) arrows: absorption (emission) lines.
emission from the receding gas. These wings should be confirmed with additional observations of H$_2$O absorption lines, as the limited wavelength coverage of the 4$_{23}$$\rightarrow$3$_{12}$ line makes the adopted baseline uncertain. The detection would indicate that H$_2$O also participates in the prominent outflow detected in OH (F10).

While the shape of the 4$_{23}$$\rightarrow$3$_{12}$ absorption line shows the centroid of the main body slightly blue-shifted (by $\sim$70 km s$^{-1}$), some lines observed in emission tend to show, on the contrary, a slight red-shift of their centroid (up to 100 km s$^{-1}$). This effect could be related to systematic motions, i.e. a low-velocity nuclear-scale outflow, and will be explored in the future with additional high spectral resolution observations.

3. Analysis

The observed pattern of line emission cannot be explained in terms of pure collisional excitation (G-A08). Adopting the collisional rates of Faure et al. (2007) with $T_k > 200$ K and $n$(H$_2$) = 10$^5$–10$^7$ cm$^{-3}$, and ignoring radiative pumping, the models that account within a factor of 2 for the high-lying 5$_{23}$$\rightarrow$5$_{12}$ and 4$_{22}$$\rightarrow$4$_{11}$ lines predict fluxes for the low-lying lines that exceed the observed values by factors of $\geq$10. Thus the observed line ratios indicate an excitation mechanism that favours the emission in the high-lying ($\gtrsim$300 K) lines at the expense of the low-lying lines.

Such a mechanism is the pumping through absorption of dust-emitted far-IR photons, which efficiently pumps the high-lying 3$_{21}$$\rightarrow$3$_{12}$/4$_{22}$$\rightarrow$4$_{11}$/5$_{23}$$\rightarrow$5$_{14}$ lines through absorptions at 75.4/57.6/45.1 $\mu$m in the strong 3$_{21}$$→$2$_{22}$/4$_{22}$$→$3$_{13}$/5$_{23}$$→$4$_{14}$ lines (Fig. 2), of which the lower backbone levels are preferentially populated. This requires a strong continuum component at 30–70 $\mu$m. However, this component cannot dominate the emission at $\gtrsim$130 $\mu$m, as it would produce strong H$_2$O absorptions in that wavelength range that are not observed (G-A08). The data then support the occurrence of both a warm/compact component with moderate opacity, and a second colder component naturally associated with the more extended 1-kpc starburst that dominates the emission at long wavelengths. Our proposed SED decomposition is shown in Fig. 3a, and defines the reference model ($M_{ref}$) with parameters as listed in Table 2: (i) a hot component (H$_C$) with $T_{dust} = 150–400$ K dominates the emission at $\lambda < 20$ $\mu$m; (ii) a warm (95 K) and compact ($R = 120$ pc) component (W$_C$) dominates at 20 $\mu$m $< \lambda < 70$ $\mu$m; (iii) an extended 1-kpc component ($E_C$), with $T_{dust} = 40$ K, accounts for most of the continuum at $\lambda > 70$ $\mu$m. The W$_C$, with $L_C \sim 1.9 \times 10^5$ L$_{\odot}$, is responsible for the observed high-lying H$_2$O line emission.

Calculations for H$_2$O were carried out using the code described in González-Alfonso & Cernicharo (1999). In $M_{ref}$ (Table 2), line broadening is caused by microturbulence. We have adopted a “mixed” approach (i.e. the H$_2$O molecules are evenly mixed with dust, G-A08), discussed below. An ortho-to-para H$_2$O abundance ratio of 3 is assumed. For those H$_2$O lines observed in emission, Fig. 3b compares the expected fluxes from the W$_C$ (in violet) with the observed fluxes (in red). Collisional excitation is included with gas at $T_k = 150$ K and $n$(H$_2$) = 1.5 $\times$ 10$^6$ cm$^{-3}$ but, even for these shock-like conditions, it has a low effect on the H$_2$O level populations and line fluxes as these are mostly determined by the strong radiation field. The high-lying lines are reproduced with the W$_C$, but there is a model deficit of emission from the low-lying lines. This deficit indicates that the $E_C$ contributes to those low-lying lines (green); both radiative and collisional excitation, the latter significant for $E_{upper} \lesssim 200$ K, are included in the model.

The high-lying 4$_{22}$$→$4$_{13}$ and 5$_{23}$$→$5$_{14}$ lines are (nearly) optically thin in the W$_C$, so that their expected fluxes are sensitive to N(H$_2$O). Table 2 shows that, despite the strong radiation field in this region, a high N(H$_2$O) is required to account for the observed fluxes. Assuming a gas-to-dust mass ratio of 100, the average H$_2$O abundance relative to H$_2$ in this W$_C$ is 0.8 $\times$ 10$^{-6}$.

The H$_2$O line at 78.7 $\mu$m observed by PACS is consistently predicted in absorption, and its flux is reasonably reproduced (Table 1), given that the blue-shifted wing is not modeled. However, the observed line shape suggests systematic motions that are not included in our model. In general, we expect that lines with $\lambda \lesssim 120$ $\mu$m are observed in absorption, while lines with $\lambda \gtrsim 120$ $\mu$m are in emission (with exceptions due to the pumping details and level energies).

Concerning the ISO lines (G-A08), $M_{ref}$ also matches the absorption in the 2$_{20}$$→$1$_{11}$ line at 101 $\mu$m, but underestimates the absorption in the 3$_{30}$$→$2$_{21}$ and 3$_{31}$$→$2$_{20}$ lines at 66.4 and 67.1 $\mu$m by a factor of 2. As mentioned above, our model uses a mixed approach, which implies that for given values of N(H$_2$O),
Table 2. Parameters of the reference model ($M_{ref}$).

<table>
<thead>
<tr>
<th>Component→</th>
<th>Hot ($T_C$)</th>
<th>Warm ($W_C$)</th>
<th>Extended ($E_C$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Radius (pc)</td>
<td>23</td>
<td>120</td>
<td>610</td>
</tr>
<tr>
<td>$T_{dust}$ (K)</td>
<td>400–150</td>
<td>95</td>
<td>41</td>
</tr>
<tr>
<td>$\tau_{100 \mu m}$</td>
<td>0.4</td>
<td>1.0</td>
<td>0.5</td>
</tr>
<tr>
<td>$L$ ($L_\odot$)</td>
<td>7.5 × 10$^3$</td>
<td>1.9 × 10$^2$</td>
<td>9.6 × 10$^3$</td>
</tr>
<tr>
<td>Gas Mass (M$_\odot$)</td>
<td>1.9 × 10$^6$</td>
<td>5.5 × 10$^6$</td>
<td>7.7 × 10$^9$</td>
</tr>
<tr>
<td>$N$(H$_2$O) (cm$^{-2}$) -</td>
<td>-</td>
<td>5.2 × 10$^{-7}$</td>
<td>2.0 × 10$^{-6}$</td>
</tr>
<tr>
<td>$V_{whb}$ (km s$^{-1}$)</td>
<td>-</td>
<td>60</td>
<td>40</td>
</tr>
<tr>
<td>$n$(H$_2$O) (cm$^{-3}$)</td>
<td>-</td>
<td>1.5 × 10$^6$</td>
<td>5 × 10$^5$</td>
</tr>
<tr>
<td>$T_{gas}$ (K)</td>
<td>-</td>
<td>150</td>
<td>100</td>
</tr>
</tbody>
</table>

Notes. (a) The hot component does not contribute to the H$_2$O emission; (b) a gas-to-dust mass ratio of 100 is assumed. (c) These parameters are not well determined for $W_C$, as the excitation is dominated by radiative pumping. (d) From Downes & Solomon (1998).

The absorbing H$_2$O lines are relatively weak, as molecules located deep inside the source do not contribute to the absorption features. Conversely, if a screen approach is adopted (i.e. a H$_2$O shell surrounds the continuum source), the absorption lines become much stronger. In both approaches, the $N$(H$_2$O) required to match the lines observed with SPIRE are similar. Thus an analysis that combines absorption and emission lines is a powerful tool to establish the distribution of H$_2$O relative to the warm dust responsible for the excitation. The screen version of $M_{ref}$ yields absorption in 3$_0$ → 2$_1$, 3$_1$ → 2$_0$, and other transitions that overestimate the observed values or upper limits. Therefore, our preliminary result is that a combination of both the mixed and screen scenarios best describes that observed data, with the mixed version favoured. Nevertheless, it remains unclear what fraction of the observed 3$_0$ → 2$_1$ and 3$_1$ → 2$_0$ absorption arises from the outflow detected in OH (F10).

By increasing $R_C$, the radius of $W_C$, to 170 pc, and keeping $L_W$ constant, the 3$_0$ → 2$_1$, 3$_1$ → 2$_0$, line strengths become overestimated by 50–25% and 25–10%; and the 2$_0$ → 2$_0$/2$_0$ → 1$_1$ intensities are underestimated by 30%; given the simplicity of our spherically symmetric models, we estimate a size for $W_C$ in the range $R_C$ = 110–180 pc. A lower limit for the luminosity arising from $W_C$ is estimated by decreasing $T_{dust}$ to 85–80 K and increasing $N$(H$_2$O) to $\geq$10$^{10}$ cm$^{-2}$, which results in too weak 4$_2$ → 3$_1$ and ISO absorption lines. We estimate that the mid- and far-IR emissions from the nuclear region account for more than 45% of the bolometric luminosity; observations at 60–200 $\mu$m are required to better constrain that value and to establish a firmer upper limit. Results are more uncertain for $E_C$, and we may expect that its contribution to the H$_2$O emission arises from its innermost region.

4. Discussion

The extreme nature of the nuclear region in Mrk 231 is well illustrated by comparing its SPIRE spectrum with that of the Orion Bar (Habart et al. 2010), the prototypical Galactic PDR. The Orion Bar spectrum shows CO lines a factor of $\geq$50 stronger than the H$_2$O lines, while in Mrk 231 the H$_2$O and CO lines have comparable strengths (vdW10). This contrast will be still higher in the nuclear region, provided that a significant fraction of the CO emission in Mrk 231 arises from a more extended region. Thus the H$_2$O-to-CO line intensity ratios in the SPIRE wavelength range are an excellent diagnostic of extragalactic compact/warm far-IR continuum sources with unusually high amounts of H$_2$O.

The above comparison also indicates that the nuclear region of Mrk 231 cannot be interpreted as an ensemble of classical PDRs. Three main scenarios are proposed to explain such high amounts of H$_2$O: (i) widespread shocks/cosmic rays: although the H$_2$O lines peak around the systemic velocity, outflows of $\sim$100 km s$^{-1}$ are not ruled out by our data, and indeed some indications in the H$_2$O line shapes of systematic motions have been found; an enhanced cosmic ray flux could also have an important impact on the nuclear chemistry. (ii) XDR chemistry: our derived H$_2$O abundance of $\sim$10$^{-6}$ is in very good agreement with XDR model results by Meijerink & Spaans (2005, their Fig. 3, Model 3), as well as with our preliminary estimate of the H$_2$O spatial distribution; (iii) an undepleted chemistry, where H$_2$O that formed on grain mantles is released into the gas phase, as in Galactic hot cores; in support of this scenario, the derived $T_{dust}$ in $W_C$ is close to the evaporation temperature of solid H$_2$O. All three scenarios are probably taking place, and the identification of the dominant process requires a multi-species analysis.

The nuclear region traced by the high-laying H$_2$O lines has a size similar to the nuclear disk (or outflow) observed at radio wavelengths and H I 21 cm by Carilli et al. (1998, their Figs. 3 and 7), suggesting a close physical correspondence. From $H_C$ and $W_C$, the nuclear surface brightness ($\sim$1.5 × 10$^{15}$ $L_\odot$ kpc$^{-2}$) exceeds the highest values attained in starburst on spatial scales $\geq$100 pc (Meurer et al. 1997; Davies et al. 2007), while the nuclear luminosity-to-mass ratio ($L/M$ $\sim$ 4 × 10$^{4}$ $L_\odot$/M$_\odot$) exceeds the limit for a starburst estimated by Scoville (2003). From near-IR data, Davies et al. (2007) estimated a starburst luminosity from a similarly sized region of $\lesssim$7 × 10$^{12}$ $L_\odot$; according to the joint luminosity of our $H_C$ and $W_C$, the AGN would account for at least 50% of the output power in Mrk 231.

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References


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