

LETTER TO THE EDITOR

First detection of the 448 GHz H₂O transition in space

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ABSTRACT

We present the first detection of the ortho-H₂O 4₂₃–3₃₀ transition at 448 GHz in space. We observed this transition in the local ($z = 0.010$) luminous infrared (IR) galaxy ESO 320-G030 (IRAS F11506-3851) using the Atacama Large Millimeter/submillimeter Array (ALMA). The water 4₂₃–3₃₀ emission, which originates in the highly obscured nucleus of this galaxy, is spatially resolved over a region of ~ 65 pc in diameter and shows a regular rotation pattern compatible with the global molecular and ionized gas kinematics. The line profile is symmetric and well fitted by a Gaussian with an integrated flux of 37.0 ± 0.7 Jy km s⁻¹. Models predict this water transition as a potential collisionally excited maser transition. On the contrary, in this galaxy, we find that the 4₂₃–3₃₀ emission is primarily excited by the intense far-IR radiation field present in its nucleus. According to our modeling, this transition is a probe of deeply buried galaxy nuclei thanks to the high dust optical depths ($\tau_{100\mu\text{m}} > 1$, $N_{\text{H}} > 10^{24}$ cm⁻²) required to efficiently excite it.

Key words. galaxies: ISM – galaxies: nuclei – infrared: galaxies – ISM: molecules

1. Introduction

Water is a molecule of astrophysical interest because it not only plays a central role in the Oxygen chemistry of the interstellar medium (e.g., Hollenbach et al. 2009; van Dishoeck et al. 2013) but it is also one of the main coolants of shocked gas (e.g., Flower & Pineau Des Forêts 2010). In addition, thanks to its energy level structure, water couples very well to the far-infrared (far-IR) radiation field providing an effective probe of the far-IR continuum in the warm compact regions found in active galactic nuclei (AGNs) and young star-forming regions (e.g., González-Alfonso et al. 2014, hereafter GA14).

Water excitation models have long predicted the maser nature of the 4₂₃–3₃₀ transition pumped by collisions when the kinetic temperature is $T_{\text{kin}} \sim 1000$ K and the hydrogen density $n_{\text{H}_2} \sim 10^5$ cm⁻³ (e.g., Deguchi 1977; Cooke & Elitzur 1985; Neufeld & Melnick 1991; Yates et al. 1997; Daniel & Cernicharo 2013; Gray et al. 2016). This transition can also be excited by radiative pumping through the absorption of far-IR photons (see Sect. 4 and Fig. 1). Therefore, the determination of the dominant excitation mechanism, which might vary from source to source, is required to properly interpret the 4₂₃–3₃₀ emission as a tracer of dense hot molecular gas or as a tracer of intense IR radiation fields in compact regions.

In this letter, we present the first detection of the ortho-H₂O 4₂₃–3₃₀ 448.001 GHz transition in space¹. No previous detections of this transition in Galactic objects have been reported,

¹ Persson et al. (2007) reported a tentative detection of the water isotopologue H₂¹⁸O 4₂₃–3₃₀ transition at 489.054 GHz in Orion, although it is blended with a much stronger methanol transition.

probably because of the high atmospheric opacity due to the terrestrial water vapor. Only recently, thanks to the sensitivity of the Atacama Large Millimeter/submillimeter Array (ALMA), it became possible to observe this transition in nearby galaxies redshifted into more accessible frequencies.

We observed the H₂O 4₂₃–3₃₀ transition in ESO 320-G030 (IRAS F11506-3851; $D = 48$ Mpc; 235 pc arcsec⁻¹). This object is an isolated spiral galaxy with a regular velocity field (Bellocchi et al. 2016) and an IR luminosity ($\log L_{\text{IR}}/L_{\odot} = 11.3$) in the lower end of the luminous IR galaxy (LIRGs) range ($11 < \log L_{\text{IR}}/L_{\odot} < 12$). It is a starburst object with no evidence of an AGN based on X-ray and mid-IR diagnostics (Pereira-Santaella et al. 2010, 2011), and hosts an extremely obscured nucleus ($A_{\text{V}} \sim 40$ mag) and a massive outflow powered by the presumed nuclear starburst detected in the ionized, neutral atomic, and molecular phases (Arribas et al. 2014; Cazzoli et al. 2014, 2016; Pereira-Santaella et al. 2016, hereafter PS16). In addition, a molecular gas inflow is suggested by the inverse P Cygni profile observed in the far-IR OH absorptions (González-Alfonso et al. 2017). It is an OH megamaser source (Norris et al. 1986), but no 22 GHz H₂O maser emission has been detected (Wiggins et al. 2016). This is consistent with the starburst activity of the nucleus of ESO 320-G030 (see Lo 2005).

2. ALMA data reduction

We obtained band 8 ALMA observations of ESO 320-G030 on 2016 November 16 using 42 antennas of the 12-m array as part of the project #2016.1.00263.S. The total on-source integration time was 10.5 min. The baselines ranged from 15 m to 920 m that

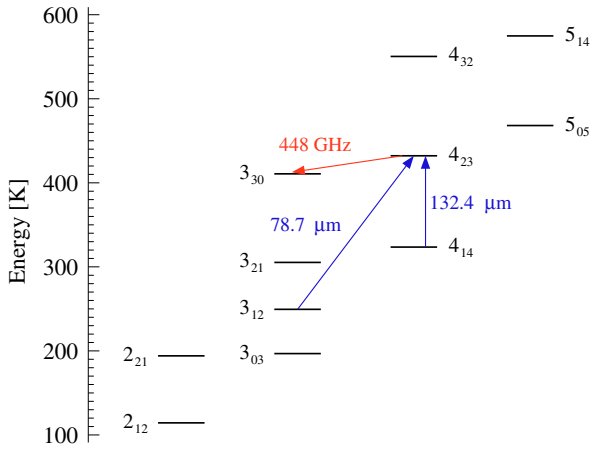


Fig. 1. Partial energy level diagram of ortho-H₂O. The 4₂₃–3₃₀ 448 GHz transition is indicated in red. The 78.7 and 132.4 μm transitions, which populate the 4₂₃ level radiatively through the absorption of far-IR photons (see Sect. 4), are marked in blue.

correspond to a maximum recoverable scale of $\sim 2''$ based on the ALMA Cycle 4 Technical Handbook equations. A three pointing pattern was used to obtain a mosaic with uniform sensitivity over a $\sim 8'' \times 8''$ field of view.

In this letter, we only use data from a spectral window centered at 443.0 GHz ($1.875 \text{ GHz}/1270 \text{ km s}^{-1}$ bandwidth and $1.95 \text{ MHz}/1.3 \text{ km s}^{-1}$ channels) where the redshifted H₂O 4₂₃–3₃₀ 448.001 GHz transition is detected. The remaining ALMA data will be analyzed in a future paper (Pereira-Santaella et al., in prep.). The data were reduced and calibrated using the ALMA reduction software CASA (v4.7.0; McMullin et al. 2007). For the flux calibration we used J1229+0203 (3C 273) assuming a flux density of 2.815 Jy at 449.6 GHz and a spectral index $\alpha = -0.78$ ($f_\nu \propto \nu^\alpha$). The final data-cube has 300×300 pixels of $0''.05$ and 31.2 MHz (20 km s^{-1}) channels. For the cleaning, we used the Briggs weighting with $R = 0.5$ (Briggs 1995) which provides a beam with a full-width half-maximum (FWHM) of $0''.26 \times 0''.24$ ($\sim 60 \text{ pc}$) and a position angle (PA) of 58° . The 1σ sensitivity is $\sim 4.8 \text{ mJy beam}^{-1}$ per channel. We corrected the data-cube for the primary beam pattern of the mosaic.

3. Data analysis

We detect continuum and line emission only in the central $\sim 200 \text{ pc}$ ($\sim 1''$). This is consistent with the extent of the 233 GHz (1.3 mm) continuum emission in this object (see PS16). We estimated the continuum level in each pixel from the median flux density in the line-free channels of the spectral window. The resulting continuum map is shown in Fig. 2. The measured total continuum emission in the central 200 pc is $183 \pm 4 \text{ mJy}$.

From the continuum subtracted data cube, we extracted the nuclear spectrum using a $d = 0''.8$ aperture (Fig. 3). A line is detected at $443451 \pm 2 \text{ MHz}$. This corresponds to a rest frame frequency of $448007 \pm 4 \text{ MHz}$ (using the systemic velocity $v_{\text{radio}} = 3049 \pm 2 \text{ km s}^{-1}$, derived from CO(2–1); see PS16) which agrees with the frequency expected for the ortho-H₂O 4₂₃–3₃₀ transition (448001 MHz; Pickett et al. 1998). This line identification is also supported by the detection of strong far-IR and sub-mm water transitions in the *Herschel* observations of this object (see Sect. 4). We also detect a weaker emission line

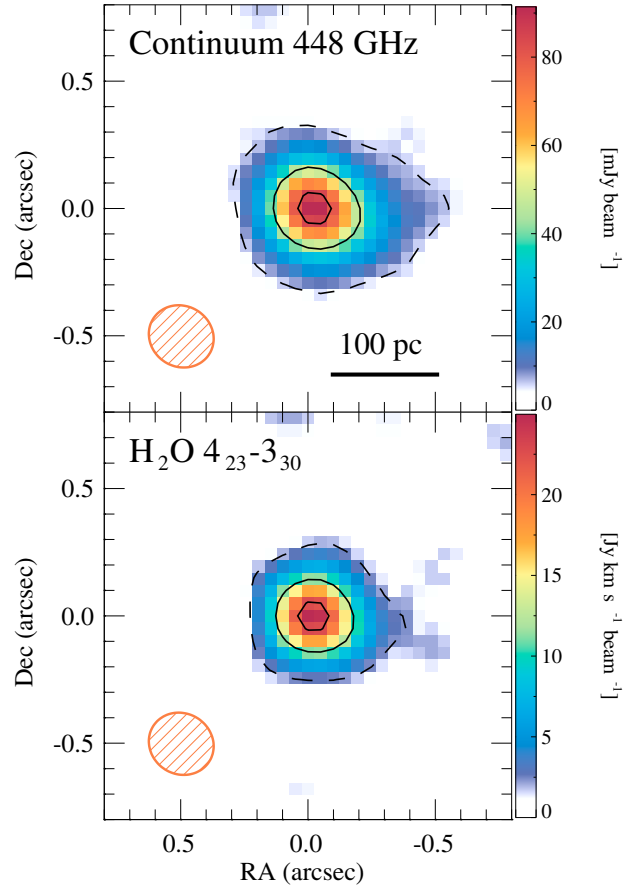


Fig. 2. Map of the 448 GHz (rest frequency) continuum (top panel) and zeroth moment of the H₂O 4₂₃–3₃₀ emission (bottom panel) of ESO 320-G030. The dashed line contour marks the 3σ level (7 mJy beam^{-1} and $2.5 \text{ Jy km s}^{-1} \text{ beam}^{-1}$, respectively). The solid contour lines indicate the peak $\times (0.5, 0.9)$ levels. The red hatched ellipses indicate the beam size ($0''.26 \times 0''.24$, PA = 58°). The coordinates are relative to $11\ 53\ 11.7192 +39\ 07\ 49.105$ (J2000).

($3.7 \pm 0.6 \text{ Jy km s}^{-1}$) which we tentatively identify as two CH₂NH transitions at $\sim 446.8 \text{ GHz}$ ($E_{\text{up}} = 96$ and 117 K ; Pickett et al. 1998). Another two CH₂NH transitions at 447.9 and 448.1 GHz might contribute to the 4₂₃–3₃₀ flux. However, these have $E_{\text{up}} \geq 280 \text{ K}$ so their contributions are likely negligible.

We fitted a Gaussian to the H₂O 4₂₃–3₃₀ profile and the result is shown in Fig. 3. We obtained a total flux of $37.0 \pm 0.7 \text{ Jy km s}^{-1}$, a velocity of $3045 \pm 1 \text{ km s}^{-1}$, and a FWHM of $161 \pm 2 \text{ km s}^{-1}$. The 4₂₃–3₃₀ profile is symmetric and it is centered at the systemic velocity. By contrast, the nuclear CO(2–1) profile has a higher FWHM and presents a more complex asymmetric profile (see Figs. 3 and 6 of PS16).

From the 448 GHz continuum and the zeroth moment water emission maps (Fig. 2), we measured the sizes of the emitting regions by fitting a 2D Gaussian. Both the continuum and the water emission are spatially resolved in the ALMA observations with the continuum being more extended. The continuum size (FWHM) is $0''.38 \times 0''.32$, which, deconvolved by the beam size, corresponds to $60 \text{ pc} \times 50 \text{ pc}$ at the distance of ESO 320-G030. The size of the water emission is $0''.30 \pm 0''.02$, which is equivalent to a deconvolved FWHM of $40 \pm 3 \text{ pc}$. For a uniform-brightness disk, the equivalent radius is $0.8 \times \text{FWHM}$ (Sakamoto et al. 2008), that is, $R \sim 45$ and $30\text{--}35 \text{ pc}$ for the 448 GHz continuum and the H₂O line, respectively.

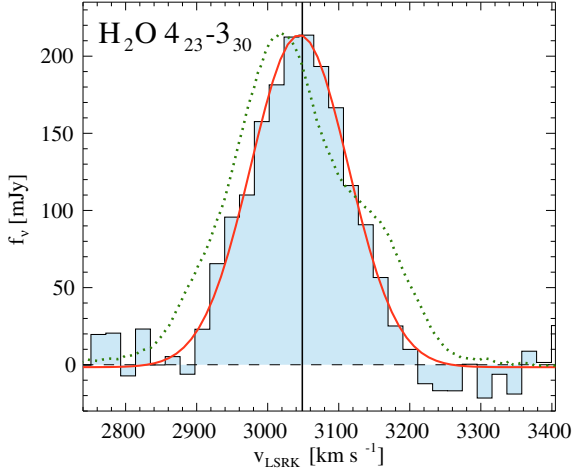


Fig. 3. Continuum subtracted profile of the $\text{H}_2\text{O } 4_{23-3_{30}}$ 448 GHz emission in ESO 320-G030 extracted using a circular aperture with $d = 0.8$ centered at the nucleus (see Fig. 2). The dotted green line is the normalized CO(2–1) profile extracted from the same region. The black vertical line indicates the systemic velocity derived from the CO(2–1) global kinematic model (PS16). The red solid line is the best Gaussian fit to the water profile (see Sect. 3).

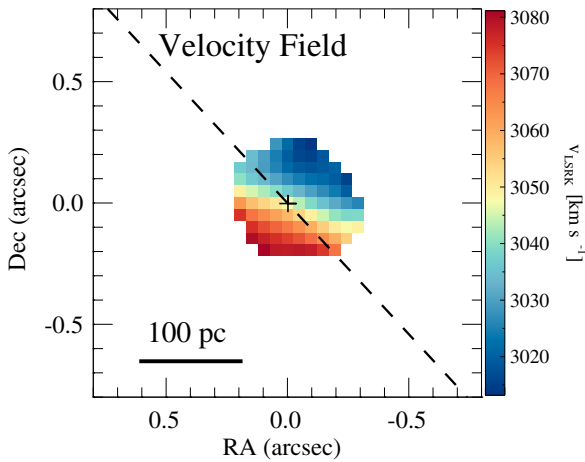


Fig. 4. Velocity field of the $\text{H}_2\text{O } 4_{23-3_{30}}$ emission. The black cross marks the position of the water emission peak (see Fig. 2). The dashed line is the minor kinematic axis derived from the kinematic analysis of the CO(2–1) emission (see PS16).

We also determined the spatially resolved kinematics of the water emission by fitting a Gaussian profile pixel by pixel. The velocity field of the water line is shown in Fig. 4 for the pixels where the line is detected at $>3\sigma$. It shows a clear rotating pattern whose kinematic axes are approximately aligned with the large-scale kinematic axes derived from both the CO(2–1) and $\text{H}\alpha$ emissions (PS16; Bellocchi et al. 2013). The slight angular deviation, $\sim 25^\circ$, is similar to that observed in the nuclear CO(2–1) kinematics and might be related to the secondary stellar bar and the elongated molecular structure associated with this bar (PS16). The FWHM line width ranges from ~ 100 – 170 km s^{-1} with the maximum value close to the water emission peak.

Based on the measured continuum fluxes at 448 GHz and 244 GHz (PS16), and on the emitting region size, we estimated the dust temperature and optical depth. First, we subtracted the free-free contribution at these frequencies ($\sim 7 \text{ mJy}$; PS16). Then, we solved the gray-body equation assuming $1.5 < \beta < 1.85$ and

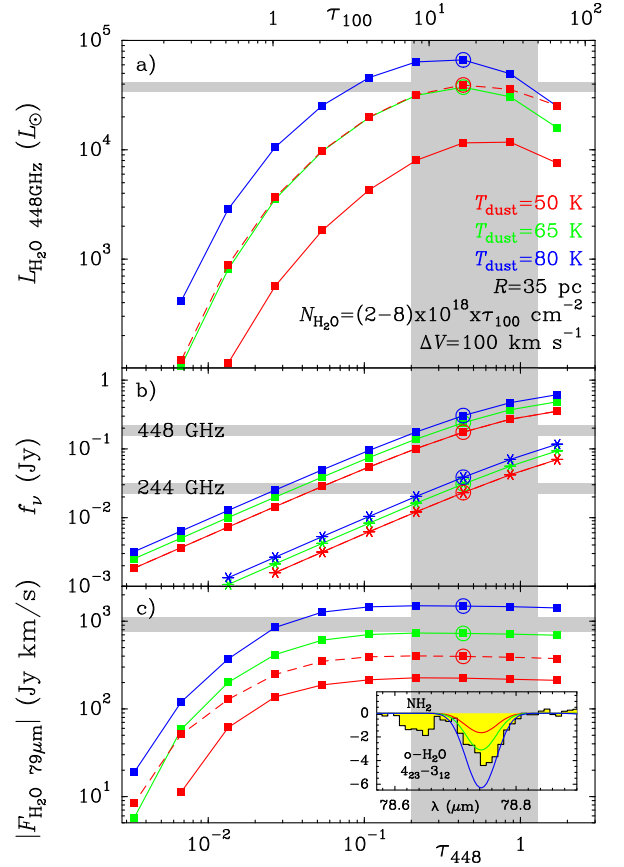


Fig. 5. a) Model predictions showing the luminosity of the $\text{H}_2\text{O } 448 \text{ GHz}$ line as a function of the continuum optical depth at 448 GHz (τ_{448} , lower axis) and at $100 \mu\text{m}$ (τ_{100} , upper axis), for uniform $T_{\text{dust}} = 50, 65,$ and 80 K . The models assume spherical symmetry with a radius $R = 35 \text{ pc}$. The assumed H_2O abundance is $X(\text{H}_2\text{O}) = 1.5 \times 10^{-6}$ (solid lines) and 6×10^{-6} (dashed red line). The shadowed regions mark the favored ranges inferred from the ESO 320-G030 observations. b) Comparison between the predicted continua at 448 GHz (squares) and 244 GHz (starred symbols) and the observed values (after subtracting the free-free emission; horizontal stripes). c) Comparison between the predicted absorbing flux of the pumping $\text{H}_2\text{O } 4_{23-3_{12}}$ line at $79 \mu\text{m}$ and the observed value ($-920 \text{ Jy km s}^{-1}$ within $\pm 150 \text{ km s}^{-1}$; horizontal stripe). The insert compares the observed $\text{H}_2\text{O } 4_{23-3_{12}}$ absorption at $78.7 \mu\text{m}$ with the predictions of the three models encircled in the three panels. The widths of the horizontal stripes assume uncertainties of $\pm 10\%$ for $L_{\text{H}_2\text{O } 448}$, and $\pm 20\%$ for the continuum flux densities and for the flux of the $\text{H}_2\text{O } 79 \mu\text{m}$ line.

using a Monte Carlo bootstrapping method to estimate the confidence intervals. We find that $T_{\text{dust}} = 25$ – 80 K and $\tau_{448 \text{ GHz}} = 0.2$ – 1.3 . These values may be significantly higher in the more compact region sampled by the $\text{H}_2\text{O } 448 \text{ GHz}$ emission.

4. Modeling the $\text{H}_2\text{O } 448 \text{ GHz}$ emission

Figure 5a shows the model predictions for the $\text{H}_2\text{O } 448 \text{ GHz}$ luminosity as a function of the continuum optical depth for different dust temperatures ($T_{\text{dust}} = 50, 65,$ and 80 K). The models, based on those reported in GA14, use the observed size ($R = 35 \text{ pc}$) and assume a H_2O column density of $N_{\text{H}_2\text{O}} = 2 \times 10^{18} \times \tau_{100}$ (solid lines) and $8 \times 10^{18} \times \tau_{100}$ (dashed red line). These values correspond to H_2O abundances relative to H nuclei of $X_{\text{H}_2\text{O}} = 1.5 \times 10^{-6}$ and 6×10^{-6} , respectively, for a standard gas-to-dust ratio of 100 by mass. The horizontal shaded

rectangle indicates the measured value of $3.8 \times 10^4 L_{\odot}$, and the vertical shaded rectangle highlights the observationally favored $\tau_{448} \gtrsim 0.2$, corresponding to $\tau_{100} \gtrsim 8$.

At low column densities, $L_{\text{H}_2\text{O}448}$ increases sharply with τ_{448} due to the enhancement of the far-IR radiation field, responsible for the H₂O excitation, and to the increase of $N_{\text{H}_2\text{O}}$. The H₂O 448 GHz line is not masing, but usually shows suprathermal excitation ($T_{\text{EX}} > T_{\text{dust}}$) in some shells.

The excitation is dominated in all cases by radiative pumping through the $4_{23}-3_{12}$ and $4_{23}-4_{14}$ lines at 78.7 and 132.4 μm (Fig. 1). Collisional excitation (included in the models with $n_{\text{H}_2} = 3 \times 10^4 \text{ cm}^{-3}$ and $T_{\text{gas}} = 150 \text{ K}$) has the effect of increasing the population of the low-lying levels from which the radiative pumping cycle works (see GA14) thus still having an overall effect on line fluxes. As τ_{100} increases above unity, the increase in τ_{100} only slightly enhances the far-IR radiation field and $L_{\text{H}_2\text{O}448}$ flattens. It is only in this regime that $L_{\text{H}_2\text{O}448}$ approaches the observed value for high enough $T_{\text{dust}} \gtrsim 65 \text{ K}$ or $N_{\text{H}_2\text{O}} = 8 \times 10^{18} \times \tau_{100}$, indicating that the H₂O 448 GHz line is an excellent probe of buried galaxy nuclei. At higher τ_{100} , line opacity effects and extinction effects at 448 GHz (for τ_{448} approaching unity) decrease $L_{\text{H}_2\text{O}448}$.

With an adopted H₂O abundance of 1.5×10^{-6} and $T_{\text{dust}} \sim 65 \text{ K}$ (green lines and symbols), we can approximately match the observed H₂O 448 GHz emission (Fig. 5a), and the 448 and 244 GHz continuum emissions (Fig. 5b) for $\tau_{448} \approx 0.3$. However, the same observables can also be fitted, for $\tau_{448} = 0.4-0.6$, with a higher $X_{\text{H}_2\text{O}} = 6 \times 10^{-6}$ and a more moderate $T_{\text{dust}} = 50 \text{ K}$ (red-dashed lines). We can discriminate between both solutions by noting that the dust opacity conditions required for the H₂O 448 GHz line to emit efficiently, $\tau_{100} > 1$, are similar to the conditions required to have strong absorption in the high-lying H₂O lines at far-IR wavelengths (e.g., González-Alfonso et al. 2012; Falstad et al. 2017), strongly suggesting that both the 448 GHz emission line and the far-IR absorption lines arise in similar regions. One of the main H₂O lines responsible for the pumping of the H₂O 448 GHz transition, the $4_{23}-3_{12}$ line at $\approx 79 \mu\text{m}$ (Fig. 1), was observed with *Herschel*/PACS (Pilbratt et al. 2010; Poglitsch et al. 2010) within the open time program HerMoLIRG (PI: E. González-Alfonso; OBSID = 1342248549). We compare in Fig. 5c the predicted absorbing flux in this line and the observed value ($-920 \text{ Jy km s}^{-1}$ between -150 and $+150 \text{ km s}^{-1}$, the observed velocity range of the H₂O 448 GHz line at zero intensity; see Fig. 3). While the $T_{\text{dust}} \sim 50 \text{ K}$ model underpredicts the pumping H₂O 79 μm absorption, the $T_{\text{dust}} \sim 65 \text{ K}$ model better accounts for it, with still some unmatched redshifted absorption (see insert in Fig. 5c). We thus conclude that the H₂O 448 GHz line originates in warm regions ($T_{\text{dust}} \gtrsim 60 \text{ K}$).

Our favored models indicate that the luminosity of the nuclear region where the H₂O 448 GHz arises is $(4-6) \times 10^{10} L_{\odot}$, that is, $\sim 25\%$ of the total galaxy luminosity. While approximately accounting for the observables reported in this Letter ($L_{\text{H}_2\text{O}448}$, allowed τ_{448} range, f_{448} , f_{244} , and $4_{23}-3_{12}$ absorption strength for the observed size), we advance the *Herschel* detection of very-high-lying H₂O absorption lines indicating the presence of an additional warmer component in the nuclear region of ESO 320-G030. The full set of H₂O (and OH) lines will be studied in a future work.

5. Conclusions

We detected the ortho-H₂O $4_{23}-3_{30}$ transition at 448 GHz using ALMA observations of the local spiral LIRG ESO 320-G030.

The H₂O 448 GHz emission arises from the highly obscured nucleus of this galaxy and is spatially resolved ($r \sim 30 \text{ pc}$). The H₂O 448 GHz velocity field is compatible with the global regular rotation pattern of the molecular and ionized gas in ESO 320-G030. Our radiative transfer modeling shows that it is mainly excited by the intense far-IR radiation field present in the nucleus of this source. The conditions for the excitation of the 448 GHz water transition indicate that it can probe deeply buried, warm environments both locally and at high redshifts.

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