First detection of the 448 GHz ortho-H$_2$O line at high redshift: probing the structure of a starburst nucleus at $z = 3.63$

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ABSTRACT

Submillimeter rotational lines of H$_2$O are a powerful probe in warm gas regions of the interstellar medium (ISM), tracing scales and structures ranging from kiloparsec disks to the most compact and dust-obscured region of galactic nuclei. The ortho-H$_2$O(4$_{23} - 3_{30}$) line at 448 GHz, which has recently been detected in a local luminous infrared galaxy, offers a unique constraint on the excitation conditions and ISM properties in deeply buried galaxy nuclei because the line requires high far-infrared optical depths to be excited. In this letter, we report the first high-redshift detection of the 448 GHz H$_2$O(4$_{23} - 3_{30}$) line using ALMA in a strongly lensed submillimeter galaxy (SMG) at $z = 3.63$. After correcting for magnification, the luminosity of the 448 GHz H$_2$O line is $\sim 10^6 L_\odot$. In combination with three other previously detected H$_2$O lines, we build a model that resolves the dusty ISM structure of the SMG, and find that it is composed of a $\sim 1$ kpc optically thin (optical depth at 100 $\mu$m $\tau_{100} \sim 0.3$) disk component with a dust temperature $T_{\text{dust}} \approx 50$ K that emits a total infrared power of $5 \times 10^9 L_\odot$, with a surface density $\Sigma_{\text{dust}} = 4 \times 10^{-11} L_\odot$ kpc$^{-2}$, and a very compact (0.1 kpc) heavily dust-obscured ($\tau_{100} \approx 1$) nuclear core with very warm dust ($100$ K) and $\Sigma_{\text{dust}} \approx 8 \times 10^{-12} L_\odot$ kpc$^{-2}$. The H$_2$O abundance in the core component, $X_{\text{H}_2\text{O}} \sim (0.3-5) \times 10^{-5}$, is at least one order of magnitude higher than in the disk component. The optically thick core has the characteristics of an Eddington-limited starburst, providing evidence that radiation pressure on dust is capable of supporting the ISM in buried nuclei at high redshifts. The multicomponent ISM structure revealed by our models illustrates that dust and molecules such as H$_2$O are present in regions that are characterized by highly differing conditions and scales, extending from the nucleus to more extended regions of SMGs.

Key words. galaxies: high-redshift – galaxies: ISM – infrared: galaxies – submillimeter: galaxies – radio lines: ISM – ISM: molecules

1. Introduction

Either in the gas phase in warm regions or locked onto dust mantles in cold environments, H$_2$O is one of the most abundant molecules in the interstellar medium (ISM). In addition to probing a variety of physical processes such as shocks (Flower & Pineau Des Forêts 2010), radiative pumping (González-Alfonso et al. 2008), and outflowing gas (van der Tak et al. 2016), it plays an essential role in the oxygen chemistry of the ISM (e.g., van Dishoeck et al. 2013). Recent observations of the rotational transitions of the H$_2$O lines in the submillimeter (submm) bands show their ubiquity in infrared (IR) bright galaxies and reveal the tight relation between the submm H$_2$O lines and dust emission (Yang et al. 2013). Case studies of local IR-bright galaxies have demonstrated that far-IR pumping plays an important role in the excitation of the H$_2$O lines (e.g., González-Alfonso et al. 2010, 2012; Liu et al. 2017). The H$_2$O lines offer diagnostics of regions of warm gas, which are usually deeply buried in dust, probing different properties of the ISM than are probed by collisionally excited lines like CO. By modeling the H$_2$O excitation, dust properties such as the dust temperature, far-IR optical depth, and IR luminosity can be constrained and can even be decomposed into multiple components that reveal the structure of the dust-obscured ISM (e.g., Falstad et al. 2015).

H$_2$O lines are a particularly powerful diagnostic tool for studying dusty galaxies. At high redshifts, such galaxies were first discovered in the submm and later characterized as submm galaxies (SMGs, e.g., Smail et al. 1997; or dusty star-forming galaxies, DSFGs, Casey et al. 2014). SMGs are undergoing massive star formation, sometimes reaching the maximum starburst limit (e.g., Barger et al. 2014). The extremely intense star formation suggests that SMGs are in the critical phase of rapid stellar mass assembly. They are likely linked to the local massive spheroidal galaxies (e.g., Toft et al. 2014). However, the nature of SMGs remains debated (e.g., Davé et al. 2010; Narayanan et al. 2015), in part due to the lack of spatially resolved studies of their dusty ISM. Hereafter, most of the H$_2$O studies at high redshifts have been based on observations with low spatial resolution, which reveal the average properties of the ISM in SMGs (e.g., Omont et al. 2013; Yang et al. 2016). Nevertheless, with ALMA, Calistro Rivera et al. (2018) have reported evidence of significant radial variation of the ISM properties in SMGs and suggested caution when interpreting single band dust continuum data. Furthermore, by measuring the structure...
of the dusty ISM, we can assess the stellar mass assembly history of SMGs and build a link to current galaxy populations (e.g., Lang et al. 2019). However, observations like this require resolving the continuum emission in multiple bands that sample the peak of the dust spectral energy distribution (SED) at high frequencies. Moreover, accessing the most dust-obscured regions is observationally challenging. The H$_2$O lines thus provide an alternative approach to constrain the structure and properties of the dusty ISM in SMGs, owing to their tight link to the far-IR radiation field.

The ortho-H$_2$O($4_{23} - 3_{30}$) line ($E_u = 433$ K) at 448.001 GHz has recently been detected for the first time in space, with the Atacama Large Millimeter/submillimeter Array (ALMA) in ESO 320-G030, an isolated IR-luminous barred spiral that is likely powered by a starburst because based on X-ray and mid-IR diagnostics, there is no evidence for an obscured active galactic nucleus (AGN; Pereira-Santaella et al. 2017). In this source, H$_2$O($4_{23} - 3_{30}$) is excited by intense far-IR radiation, rather than being a maser line, as predicted by collisional models (e.g., Neufeld & Melnick 1991; Gray et al. 2016). The spatially resolved observations of the H$_2$O($4_{23} - 3_{30}$) line and dust continuum in ESO 320-G030 indicate that the line arises from a highly obscured galactic nucleus. Therefore, this highly excited H$_2$O line is an ideal probe of the deeply buried (optically thick in the far-IR), warm dense nuclear ISM of galaxies.

In this Letter, we report the first high-redshift detection of the ortho-H$_2$O($4_{23} - 3_{30}$) line in a strongly lensed SMG at $z = 3.63$ in the SMG merging pair G09v1.97. It was first discovered with Herschel (Bussmann et al. 2013) and was followed up with observation of low spatial resolution of several H$_2$O and CO lines (Yang et al. 2016, 2017) and a high-resolution observation of the H$_2$O($2_{11} - 2_{02}$) and CO(6–5) lines (Yang et al. 2019, Y19 hereafter). G09v1.97 has a total molecular gas mass of $10^{11} M_{\odot}$, and is composed of two gas-rich merging galaxies. The two galaxies, dubbed G09v1.97-R (the receding northern galaxy) and G09v1.97-B (the approaching southern galaxy), are separated by a projected distance of 1.3 kpc ($\sim 9.2''$) and have total intrinsic IR luminosities (8–1000 µm) of $6.3 \times 10^{12}$ and $4.0 \times 10^{12} L_{\odot}$, respectively. While both G09v1.97-R and G09v1.97-B are one order of magnitude more powerful than ESO 320-G030 in IR luminosity, like ESO 320-G030, these galaxies are likely powered by star formation, based on their similar line-to-IR luminosity ratios of $L_{\text{CO(6–5)}}/L_{\text{IR}}$ and $L_{\text{H}_2\text{O}(2_{11}–2_{02})}/L_{\text{IR}}$ (Yang et al. 2013, Y19).

We adopt a spatially flat ΛCDM cosmology with $H_0 = 67.8 \text{ km} \text{s}^{-1} \text{Mpc}^{-1}$, $\Omega_M = 0.308$ (Planck Collaboration III 2016), and a Chabrier (2003) initial mass function (IMF) throughout this work.

### 2. Observations and data reduction

The ALMA observations presented here are part of a dense gas line survey project (ADS/JAO.ALMA#2018.1.00797.S, Yang et al., in prep.). The observations were carried out between December 2018 and January 2019. In this work, we only present data from the Band-3 spectral window covering the ortho-H$_2$O($4_{23} - 3_{30}$) line centered at 96.137 GHz (observed frequency). Forty-three antennas of the 12 m array were used. The observations were performed under good weather conditions (PWV $\approx 2–5$ mm, phase RMS $< 9''$) with the C43-2 configuration, which provides baselines ranging from 15 to 200 m. J0825+0309 was used as the phase calibrator and J0750+1231 as the bandpass and flux calibrator. A typical ALMA Band-3 calibration uncertainty of 5% is adopted. The total on-source time was 118.4 min, with an additional overhead time of 47.7 min, resulting in a sensitivity of $\sim 0.12$ mJy beam$^{-1}$ in 50 km s$^{-1}$ velocity bins.

The data were calibrated using the ALMA calibration pipelines with minor flagging. The calibrated data were further processed with imaging and CLEANing using the tclean procedure of the CASA software (McMullin et al. 2007) version 5.4.0, with a natural weighting (synthesis beam size of 2.46$'' \times 2.03''$ and PA = 78.2$'$) to maximize the signal-to-noise ratio. The beam size is unable to resolve the source, which has a largest angular structure of $\sim 2''$ (Y19). The spectrum was then extracted from the spatially integrated emission over the entire source (Fig. 1).

### 3. Analysis and discussion

As shown by the high-angular resolution observations in Y19, the CO(6–5) and H$_2$O($2_{11} – 2_{02}$) lines of G09v1.97 both mainly consist of B and R components (which are blueshifted and redshifted, respectively, compared to the system velocity of G09v1.97), with line widths of $\sim 300$ km s$^{-1}$ (Fig. 1). The B component originates exclusively from the approaching galaxy G09v1.97-B, while the R component arises from the receding galaxy G09v1.97-R. Therefore, the contribution to the spectrum from each merger companion can be distinguished without spatially resolved observations. The lensing magnification for the line varies from $\sim 5$ to $\sim 22$ as a function of velocity from the blueshifted to the redshifted velocity components, due to a velocity gradient from south to north (Y19). As a result, R is a factor of $\gtrsim 4$ brighter than B in the spectrum, causing an extremely asymmetric line profile (blue histogram in Fig. 1). The 448 GHz H$_2$O line is detected with $\gtrsim 5$σ significance, but only in the redshifted component (Fig. 1), namely only in G09v1.97-R. Assuming a similar flux ratio of H$_2$O($4_{23} - 3_{30}$)/H$_2$O($2_{11} – 2_{02}$) in R and B, the 448 GHz H$_2$O line in G09v1.97-B is thus buried below the noise level. Therefore, we associate the detected 448 GHz H$_2$O line only with G09v1.97-R. We therefore corrected the lensing magnification for the H$_2$O line fluxes of G09v1.97-R, as listed in Table 1. The table also includes the observational results on the H$_2$O($3_{21} – 3_{12}$) (Yang et al. 2016) and H$_2$O($4_{23} – 4_{13}$) lines (Yang 2017) for G09v1.97-R, which were obtained with

![Fig. 1. Spatially integrated spectrum of the 448 GHz H$_2$O line of G09v1.97 (yellow histograms). B and R correspond to the blue- and redshifted components of G09v1.97. The overlaid blue line shows the observed H$_2$O($2_{11} – 2_{02}$) line (Y19) after scaling its flux density down by a factor of 25. The dashed red lines show Gaussian fitting to the emission lines. Close to the 448 GHz H$_2$O line, we also tentatively detect a 2.3σ emission line (at the velocity of the R component) at $\sim 449$ GHz, which may be either C$^1$O(4–3) or c-C$_3$H$_2$(762 – 651). If the emission is indeed C$^1$O(4–3), the integrated flux density ratio of C$^1$O(4–3)/C$^1$O(4–3) would be $\sim 110$, which will be discussed in Yang et al. (in prep.). The dust continuum at rest frame 615 mJy is also detected with a flux density of 1.13 ± 0.04 mJy.](https://example.com/figure1.png)
The continuum measurements, which are used below to model the H$_2$O emission, were also corrected to account for G09v1.97-R alone. The limited spatial resolution of the currently highest spatial resolution dust continuum images (Y19) does not allow us to distinguish the fluxes from the merger companions. Nevertheless, the relative contribution by G09v1.97-R can be approximated using the tight correlation between LCO(6–5) and L$_{IR}$ (Liu et al. 2015; Yang et al. 2017). Because the intrinsic line fluxes from R are about 50% of the total and the magnifications R and B are $\mu_R \approx 20$ and $\mu_B \approx 5$, respectively (Y19), the intrinsic continuum flux densities from G09v1.97-R are a factor $\approx 25$ lower than the observed values integrated over the entire G09v1.97 system. We here therefore scaled the measured continuum fluxes down by a factor of 25 and include an uncertainty of 20% associated with the flux scaling.

In G09v1.97-R, the 448 GHz ortho-H$_2$O($43_2 - 33_0$) line has a luminosity of 8.5 $\times$ 10$^3$ L$_{\odot}$, which is a fraction of 10$^{-6}$ of the total IR luminosity. In addition to the 448 GHz H$_2$O line, three additional lines of H$_2$O have previously been detected in G09v1.97-R (Fig. 2 and Table 1): the ortho-H$_2$O($3_{21} - 3_{12}$), the para-H$_2$O($2_{11} - 2_{02}$), and the para-H$_2$O($4_{32} - 4_{31}$) transitions. Interestingly, the $4_{32} - 3_{30}$ and $4_{22} - 4_{13}$ transitions have $J_{\text{upper}} = 4$ levels with very similar energies (425 K versus 433 K), but their A-Einstein coefficients for spontaneous emission differ by a factor of $\approx 500$, 5.4 $\times$ 10$^{-10}$ and 2.8 $\times$ 10$^{-11}$, respectively (Pickett et al. 1998). Assuming that the upper-level populations of both lines do not strongly differ from the ortho-to-para ratio of 3 appropriate for warm regions, their flux ratio (in Jy km s$^{-1}$) in optically thin conditions should be $F(1208\text{GHz})/F(448\text{GHz}) \approx A_{u}(1208\text{GHz})/A_{u}(448\text{GHz}) \approx 170$. The observed flux ratio in G09v1.97-R is only $\approx 11$ (Table 1), similar to the value of $\approx 15$ found in ESO 320-G030 (González-Alfonso et al., in prep.), indicating that the ortho-H$_2$O($4_{32} - 4_{31}$) line is strongly saturated in both sources. Similar to the situation found in buried nuclei of local (ultra-)luminous IR galaxies (U)LIRGs, high radiation and column densities in a nuclear component are required to pump the $J_{\text{upper}} = 4$ levels and to account for the corresponding strong H$_2$O emission from G09v1.97-R.

To estimate the physical conditions and structure of the ISM in G09v1.97-R from the observed H$_2$O and dust continuum emission, a library of model components was developed following the method described in González-Alfonso et al. (2014). We assumed for each component a spherically symmetric source with uniform physical properties: the dust temperature $T_{\text{dust}}$, the continuum optical depth at 100 $\mu$m along a radial path $\tau_{100}$, the column density of H$_2$O along a radial path $N_{\text{H}_2\text{O}}$, the H$_2$ density $n_{\text{H}_2}$, the velocity dispersion $\Delta V$, and the gas temperature $T_{\text{gas}}$.

The physical parameters modified from model to model are $T_{\text{dust}}$, $\tau_{100}$, $N_{\text{H}_2\text{O}}$, and $n_{\text{H}_2}$, and we kept $\Delta V = 100$ km s$^{-1}$ and $T_{\text{gas}} = 150$ K fixed (consistent with the results from CO excitation, Yang et al. 2017). The model components were classified into groups according to their physical parameters, each group covering a regular grid in the parameter space ($T_{\text{dust}}$, $\tau_{100}$, $N_{\text{H}_2\text{O}}$, and $n_{\text{H}_2}$). After we created the model components, all available H$_2$O line fluxes and continuum flux densities were fit simultaneously using a number $N_{\text{c}}$ of model components (up to two components per group) and checking all possible combinations among them. Because the intrinsic line and continuum fluxes (in Jy km s$^{-1}$ and $\mu$Jy, respectively) scale as $(1+z)(R/D)\gamma$, where $R$ is the source radius and $D_L = 32.7$ Gpc is the luminosity distance, a $\chi^2$ minimization procedure was used to determine the source radius $R$ of each component for all combinations of model components. Our best model fit corresponds to the combination that yields the lowest $\chi^2$, while the results for all combinations enable us to calculate the likelihood distribution of the free physical parameters (e.g., Ward et al. 2003), i.e., $T_{\text{dust}}$, $\tau_{100}$, $N_{\text{H}_2\text{O}}$, and $n_{\text{H}_2}$, for each component. The derived parameters ($R$, the H$_2$O abundance relative to H nuclei $X_{\text{H}_2\text{O}}$, and $L_{IR}$) can also be inferred. More details will be given in González-Alfonso et al. (in prep.).

We first attempted to fit the H$_2$O and continuum emission with a single-model component ($N_{\text{c}} = 1$), but results were unreliable, with a best reduced chi-square value $\chi^2_{\text{red}}$ $\approx 4$. This was indeed expected because the low-lying H$_2$O $J_{\text{upper}} = 2$–3 lines are expected to arise in more extended regions than the $J_{\text{upper}} = 4$ lines that trace buried regions (e.g., González-Alfonso et al. 2014; Pereira-Santaella et al. 2017). A better fit was found...
with $N_C = 2$ components (Fig. 3), with $\chi^2_{\text{red}} \approx 0.9$. In Fig. 4, the arrows indicate the best-fit values, and solid histograms show their likelihood distributions. We find that the $J_{\text{upper}} = 4$ lines are formed in a very warm nuclear region (core) with size $R \sim 100 \, \text{pc}$ and $T_{\text{dust}} \sim 100 \, \text{K}$, which is most probably optically thick at far-IR wavelengths ($\tau_{100} \gtrsim 1$). This nuclear core has a luminosity of $L_{\text{IR}} \sim 10^{12} L_{\odot}$, resulting in an extreme IR luminosity surface density $\Sigma_{\text{IR}} \approx 8 \times 10^{-2} L_{\odot} \, \text{kpc}^{-2}$. This translates into a surface star formation rate of $\sim 1.1 \times 10^3 M_{\odot} \, \text{yr}^{-1} \, \text{kpc}^{-2}$ if the contribution to $L_{\text{IR}}$ by a possible obscured AGN is negligible because no strong evidence of the presence of an AGN has been found (Yang et al. 2016). A high column density of water, $N_{\text{H}_2\text{O}} \sim 10^{19} \, \text{cm}^{-2}$ ($X_{\text{H}_2\text{O}} \sim 10^{-3}$), is found in this core component, which is more than one order of magnitude higher than in the $z = 3.9$ quasar host galaxy APM08279+5255 (van der Werf et al. 2011). In addition, the $J_{\text{upper}} = 2-3$ lines, pumped by absorption of dust-emitted 100 and 75 $\mu$m photons (Fig. 2), require an optically thin ($\tau_{100} \sim 0.3$) and more extended region of radius $\sim 1 \, \text{kpc}$ (the disk component), remarkably similar to the projected half-light effective radius traced by the CO(6–5) and H$_2$O($2_{11} - 2_{02}$) line emission (0.8 kpc, Y19), and also to the size of the averaged 870 $\mu$m dust continuum of SMGs ($\sim 1 \, \text{kpc}$, Gullberg et al. 2019). With $T_{\text{dust}} \sim 50 \, \text{K}$, the disk component dominates the luminosity with $L_{\text{IR}} \sim 5 \times 10^{11} L_{\odot}$ and $\Sigma_{\text{IR}} = 4 \times 10^{11} L_{\odot} \, \text{kpc}^{-2}$ (corresponding to $\sim 60 M_{\odot} \, \text{yr}^{-1} \, \text{kpc}^{-2}$), and has a lower column density and abundance of water than the core, with $N_{\text{H}_2\text{O}} \sim 10^{18} \, \text{cm}^{-2}$ ($X_{\text{H}_2\text{O}} \sim 10^{-4}$).

While the effect of the cosmic microwave background (CMB) on the dust SED is included in Fig. 3b following da Cunha et al. (2013) (see also Zhang et al. 2016), the correction is small as $T_{\text{dust}} \gg T_{\text{CMB}} = 12.5 \, \text{K}$. The excitation of H$_2$O by the CMB, however, is not included in our models, but we verified that for our best-fit model (Fig. 3a), it has a negligible effect on the excitation and flux of the observed lines. A more important source of uncertainty is that our models do not include the effects of spatially varying $T_{\text{dust}}$ that are expected in regions that are optically thick in the far-IR (González-Alfonso & Sakamoto 2019). An increasing $T_{\text{dust}}$ outside-in would facilitate the H$_2$O excitation within the core component, and would thus decrease the inferred $N_{\text{H}_2\text{O}}$ to some extent. This effect becomes most relevant for extremely buried sources with $N_{\text{H}_2\text{O}}$ approaching $10^{25} \, \text{cm}^{-2}$ ($\tau_{100} \gtrsim 10$), which is not excluded for the nuclear core of G09v1.97-R (Fig. 4b).

What is the role of the 448 GHz H$_2$O line in constraining the model? The dotted histograms in Fig. 4 show that if the 448 GHz H$_2$O line is excluded, the likelihood distributions of the physical parameters remain similar, but show a less informative distribution for $N_{\text{H}_2\text{O}}$ (and $X_{\text{H}_2\text{O}}$). In this case, the parameters of the nucleus are determined by the 1208 GHz H$_2$O line, which is optically thick ($\tau_{1208-\text{H}_2\text{O}} = 27.5$). The detection of the more optically thin 448 GHz H$_2$O line (T$_{\text{448-H}_2\text{O}} = 1.0$) confirms the occurrence of the warm nuclear region and enables a significantly more accurate estimate of its $N_{\text{H}_2\text{O}}$ (and $X_{\text{H}_2\text{O}}$). On the other hand, the flat distributions of $n_{\text{H}_2}$ in both regions
indicate that the excitation of these H$_2$O lines is insensitive to $n_{H_2}$.

Our models, which fit the H$_2$O line and dust continuum fluxes simultaneously, are sensitive to $N_{H_2}$ and $T_{100}$. These two parameters, treated as independent, are linked as $X_{H_2} = N_{H_2}/(1.3 \times 10^{24} T_{100} (GDR/100))$, where GDR is the gas-to-dust ratio by mass. For the core component, our best fit yields $N_{H_2}/T_{100} = 5 \times 10^{18}$ cm$^{-2}$. With a assumption of $GDR = 100$, we obtain $X_{H_2}$ $\sim (0.3-5) \times 10^{-2}$ (90% confidence interval, Fig. 4e), similar to the abundance in buried galactic nuclei of local (U)LIRGs (González-Alfonso et al. 2012). The similarity of the $N_{H_2}/T_{100}$ ratio in the nuclear cores of SMGs and of local (U)LIRGs appears to indicate a fundamental similarity of the gas metallicity to dust ratio in buried galactic nuclei throughout cosmic times.

With the H$_2$O excitation models, we are able to resolve two distinct components with significantly different properties (e.g., $T_{\text{dust}}$ and $T_{100}$). These differences reveal the complexity of the ISM ~tripe-opt SMG thin ($T_{100} < 0.3$) disk component with $T_{\text{dust}} = 50$ K emitting a total IR luminosity of $5 \times 10^{12} L_{\odot}$, and a $\sim 0.1$ kpc heavily dust-obscured ($T_{100} \geq 1$) nuclear core with very warm dust (100 K) and an IR luminosity of $\sim 10^{12} L_{\odot}$. The water abundance in the core ($X_{H_2} \sim 5 \times 10^{-6}$) is more than one order of magnitude higher than in the more extended disk. The spatial surface flux ratio of the core component is $\Sigma_{\text{SFR}} = 1.1 \times 10^{15} M_\odot \text{yr}^{-1} \text{kpc}^{-2}$, which is $\sim 20$ times higher than that of the disk. The ISM properties of the nucleus of G09v1.97-R resemble the characteristic properties of an Eddington-limited starburst, indicating that radiation pressure on dust plays an essential role in supporting the ISM.

The optically thin 448 GHz H$_2$O line is a powerful tool for the study of SMGs around redshift 2–4 (with ALMA Bands 3 and 4). The multicomponent structure derived from the H$_2$O excitation model reveals the complex nature and morphology of SMGs and may offer clues about the evolutionary link of the SMGs to massive elliptical galaxies today, once high-resolution near-infrared observations of the stellar component are possible and become available with telescopes such as the James Webb Space Telescope, JWST.

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