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## Probing the full CO spectral line energy distribution (SLED) in the nuclear region of a quasar-starburst system at $z = 6.003$

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### ABSTRACT

We report Atacama Large Millimeter/submillimeter Array (ALMA) observations of CO (8 – 7), (9 – 8), H<sub>2</sub>O(2<sub>0,2</sub> – 1<sub>1,1</sub>) and OH<sup>+</sup>(1<sub>1</sub> – 0<sub>1</sub>) and NOEMA observations of CO (5 – 4), (6 – 5), (12 – 11) and (13 – 12) towards the  $z = 6.003$  quasar SDSS J231038.88+185519.7, aiming to probe the physical conditions of the molecular gas content of this source. We present the best sampled CO spectral line energy distribution (SLED) at  $z = 6.003$ , and analyzed it with the radiative transfer code MOLPOP-CEP. Fitting the CO SLED to a one-component model indicates a kinetic temperature  $T_{\text{kin}} = 228$  K, molecular gas density  $\log(n(\text{H}_2)/\text{cm}^{-3}) = 4.75$ , and CO column density  $\log(N(\text{CO})/\text{cm}^{-2}) = 17.5$ , although a two-component model better fits the data. In either case, the CO SLED is dominated by a ”warm” and ”dense” component. Compared to samples of local (Ultra) Luminous Infrared Galaxies ((U)LIRGs), starburst galaxies and high redshift Submillimeter Galaxies (SMGs), J2310+1855 exhibits higher CO excitation at ( $J \geq 8$ ), like other high redshift quasars. The high CO excitation, together with the enhanced  $L_{\text{H}_2\text{O}}/L_{\text{IR}}$ ,  $L_{\text{H}_2\text{O}}/L_{\text{CO}}$  and  $L_{\text{OH}^+}/L_{\text{H}_2\text{O}}$  ratios, suggests that besides the UV radiation from young massive stars, other mechanisms such as shocks, cosmic rays and X-rays might also be responsible for the heating and ionization of the molecular gas. In the nuclear region probed by the molecular emissions lines, any of these mechanisms might be present due to the powerful quasar and the starburst activity.

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## 1. INTRODUCTION

The quasars discovered at  $z \gtrsim 6$  represent the first generation of super massive black holes (SMBHs) and host galaxies. Many among these earliest systems host SMBHs of  $\sim 10^9 M_\odot$  (e.g., Jiang et al. 2007, 2016), and the strong dust continuum and [C II] detections reveal dynamical masses of  $\sim 10^{10} - 10^{11} M_\odot$  and star formation rate of  $\sim 10^2 - 10^3 M_\odot \text{ yr}^{-1}$  in the host galaxies (e.g., Maiolino et al. 2005; Wang et al. 2008, 2016, 2019; Walter et al. 2009; Carilli & Walter 2013; Venemans et al. 2017, 2019; Decarli et al. 2018; Neeleman, et al. 2019). These suggest that the SMBH and galaxy co-evolution is already in place in these  $z \sim 6$  quasar-starburst systems. In the meantime, bright molecular CO emission lines are widely detected in the starburst quasar hosts which reveal the molecular gas content of  $\sim 10^9 - 10^{10} M_\odot$  within a few kpc scale (e.g., Bertoldi et al. 2003; Walter et al. 2003; Riechers et al. 2009; Wang et al. 2010, 2011, 2013, 2016; Carilli & Walter 2013; Venemans et al. 2017). In particular, the  $z \gtrsim 6$  quasars are detected in very high (rotational quantum number)  $J$  (e.g.,  $J \gtrsim 9$ ) CO transitions, indicating high CO excitation comparable to that found in local extreme (Ultra)luminous Infrared Galaxies ((U)LIRGs) and AGNs (e.g., Gallerani et al. 2014; Wang et al. 2019; Yang et al. 2019). Taking the advantage of the most powerful sub-mm/mm and radio facilities, such as Atacama Large Millimeter/submillimeter Array (ALMA), NOthern Extended Millimeter Array (NOEMA) and the Karl G. Jansky Very Large Array (VLA), extensive observations at submm/mm wavelengths have recently been carried out to search for the emission lines from the ionized, atomic, and molecular interstellar medium (ISM) (e.g., Decarli et al. 2018; Hashimoto et al. 2018; Walter et al. 2018; Novak et al. 2019). These observations are crucial for our understanding of the physical, chemical conditions and kinematics of the multi-phase ISM in these young quasar hosts at the earliest epoch and allow us to study the co-evolution of SMBHs and their host galaxies at the earliest evolutionary phase.

CO emission lines have long been the workhorse to probe the molecular gas at rest-frame sub-mm band in the local and high redshift Universe. Low  $J$  (e.g.,  $J \lesssim 3$ ) CO emission lines are easy to excite in typical molecular cloud conditions (i.e., the lowest CO transition requires only  $\sim 5$  K above ground and densities of  $\sim 100 \text{ cm}^{-3}$ ), thus it traces the bulk of the molecular gas content. Mid  $J$  (e.g.,  $4 \lesssim J \lesssim 8$ ) CO transitions are found to be linearly correlated with the far infrared luminosity and trace the star formation rate (e.g., Greve et al. 2014; Liu et al. 2015). UV photons from newly formed high-mass stars are responsible for the molecular gas heating at this regime. The excitation of high  $J$  (e.g.,  $J \gtrsim 9$ ) CO transitions require both high temperature and high density, which are usually related to the processes such as shocks, X-rays from AGN and cosmic rays (Bradford et al. 2003; Spinoglio et al. 2012; Meijerink et al. 2013; Gallerani et al. 2014).

CO spectral line energy distribution (SLED) – the CO flux as a function of rotational quantum number  $J$  is a probe of the molecular gas physical conditions (e.g., temperature, density and illuminating radiation field strength). It has been used to study the physical conditions in a variety of local and high redshift systems (e.g., Weiß et al. 2005, 2007; Riechers et al. 2006; Bradford et al. 2009, 2011; Spinoglio et al. 2012; Gallerani et al. 2014; Yang et al. 2019; Wang et al. 2019). Normal star-forming galaxies have CO SLEDs that peak at relatively low  $J$  CO transitions. E.g., the CO SLED of the Milky Way’s inner disk peaks at around  $J = 3 - 4$  (Fixsen et al. 1999), and similar CO SLEDs are found in other local star-forming galaxies (Daddi et al. 2015). Galaxies that experience higher star formation activity than normal galaxies, e.g., starburst galaxies, (U)LIRGs and submillimeter galaxies (SMGs), have moderately excited CO SLEDs which peak at higher  $J$  compared to the star forming galaxies. One of the closest examples is the local starburst galaxy M82, whose CO SLED peaks at  $J = 5$  in the central region and show little line intensity at  $J > 9$  (Weiß et al. 2005; Panuzzo et al. 2010). The molecular CO in luminous AGNs are usually highly excited. Very high  $J$  CO transitions ( $J \gtrsim 9$ ) are detected in well-known AGNs such as NGC 1068 (Spinoglio et al. 2012), Mrk231 (van der Werf et al. 2010), the Cloverleaf quasar at  $z = 2.56$  (Bradford et al. 2009; Uzgil et al. 2016) and the  $z = 3.9$  lensed quasar APM 08279+5255 (Weiß et al. 2007; Riechers et al. 2009; Bradford et al. 2011). And known to date, bright CO emission lines at  $J \geq 10$  were detected in the host galaxies of three  $z \geq 6$  quasars, i.e., SDSS J114816.64+525150.3 (here after J1148+5251) at  $z = 6.4$  (e.g., Riechers et al. 2009; Gallerani et al. 2014), SDSS J010013.02+280225.8 (here after J0100+2802) at  $z = 6.3$  (Wang et al. 2019) and UHS J043947.08+163415.7 (hereafter J0439+1634) at  $z = 6.5$  (Yang et al. 2019). The CO lines at  $J \geq 10$  are likely to arise from warm gas with kinetic temperature of  $T_{\text{kin}} \geq 100$  K. Kinetic temperature is proportional to the kinetic energy through  $T_{\text{kin}} = \frac{2}{3} \frac{E_n}{k_B}$ , where  $k_B$  is Boltzmann constant

and  $E_n$  is the kinetic energy of the molecule. In the high redshift quasars, X-rays from AGNs are frequently proposed to explain the CO excitation at high  $J$  transitions (Bradford et al. 2009; Gallerani et al. 2014; Uzgil et al. 2016).

The  $\text{H}_2\text{O}$  and  $\text{OH}^+$  lines provide additional diagnostics of heating and ionization source of the molecular gas (e.g., Cosmic rays, UV radiation, X-rays and shocks) in addition to CO. The  $\text{H}_2\text{O}$  molecule traces the warm and dense molecular regions. It is found to be bright in infrared luminous galaxies, and can even reach luminosities comparable to CO in these galaxies (van der Werf et al. 2011; Omont et al. 2013; Yang et al. 2013, 2016; Jarugula et al. 2019). Recent studies found a nearly linear relation between the water luminosity and the infrared luminosity in local and high redshift systems over three orders of magnitude (González-Alfonso et al. 2010; ?; Riechers et al. 2013; Yang et al. 2013, 2017; Omont et al. 2013; Jarugula et al. 2019). The brightest water lines are detected in the presence of shocks or X-rays (González-Alfonso et al. 2010; Pellegrini et al. 2013). Accordingly, the  $\text{H}_2\text{O}$  emission may even act as a tracer of the powering source of molecular gas, e.g., if the molecular gas is heated by the UV radiation or other mechanisms like shocks and X-rays. In addition, a variety of chemical processes are enrolled in the formation of  $\text{H}_2\text{O}$  and  $\text{OH}^+$ . The gas phase  $\text{H}_2\text{O}$  molecule is formed by either solid-phase or gas-phase chemical reactions (Pellegrini et al. 2013; Yang et al. 2016). Neutral-neutral and ion-neutral reactions are two mechanisms to form  $\text{H}_2\text{O}$  molecule in the gas phase. The former is usually related to the shocks, while the later is associated with PDRs, cosmic ray dominated regions, and X-ray dominated regions (Yang et al. 2016). The molecular ions (e.g.,  $\text{H}_2\text{O}^+$ ,  $\text{OH}^+$ ) as intermediates of the ion-neutral reactions, play important roles in distinguishing between shocks and PDR/XDR/cosmic ray dominated region. E.g., the bright  $\text{H}_2\text{O}^+$  line detection in high redshift lensed SMGs is probably initiated by cosmic rays (Yang et al. 2016).

The  $\text{OH}^+$  line, although not as strong as the turbulent gas tracer  $\text{CH}^+$  that has been detected in high redshift systems (e.g., Falgarone et al. 2017), traces the turbulent gas components as well, e.g., inflow or outflows. The formation of  $\text{OH}^+$  requires both atomic and molecular hydrogen, at which column density the cosmic-rays or X-rays are more capable of penetrating and ionizing the neutral and molecular gas (e.g., van der Werf et al. 2010; Meijerink et al. 2011; González-Alfonso et al. 2018). The  $\text{OH}^+$  line has been detected both in absorption (that probes the cold turbulent gas) and in emission, where the chemical structure is dominated by the cosmic ray ionization or the X-ray radiation from the AGNs (e.g., van der Werf et al. 2010; González-Alfonso et al. 2018). Limited by the weak strength and the P Cygni line profile (presence of both absorption and emission in the profile of the same spectral line), there is only one reported  $\text{OH}^+$  line detection at  $z \geq 6$  in absorption in the starburst galaxy HFLS3 (Riechers et al. 2013).

In order to understand the physical conditions and the heating mechanisms of the ISM in the complex environment with both AGN and nuclear starburst activities in these young quasar hosts at  $z \sim 6$ , we here present a study of the CO SLED in one of the most far infrared and CO luminous quasars at  $z \sim 6$ , SDSS J231038.88+185519.7 (here after J2310+1855) at  $z = 6.003$ . J2310+1855 hosts a SMBH of  $\approx 4 \times 10^9 M_\odot$  (Jiang et al. 2016). It was detected in bright dust continuum, CO (2 – 1) and (6 – 5), [C II]  $158\mu\text{m}$  and [O III]  $88\mu\text{m}$  lines (Wang et al. 2013; D’Odorico et al. 2018; Feruglio et al. 2018; Hashimoto et al. 2018; Carniani et al. 2019; Shao et al. 2019). This quasar is also detected in bright CO (10 – 9) emission with a line flux of  $1.04 \pm 0.17 \text{ Jy km s}^{-1}$  (Riechers et al. in prep). The far infrared dust emissions suggest the host galaxy is actively forming stars with a star formation rate (SFR) of  $\approx 2400 M_\odot \text{ yr}^{-1}$ , and is abundant in dust with a dust mass of  $\approx 1.7 \times 10^9 M_\odot$  (Wang et al. 2013; Hashimoto et al. 2018; Carniani et al. 2019; Shao et al. 2019). Wang et al. (2013) for the first time spatially resolved the large amount of gas ( $\approx 9.6 \times 10^{10} M_\odot$ ) residing in a  $0''.55 \times 0''.40$  ( $\sim 3 \text{ kpc}$ ) disk based on the [C II]  $158\mu\text{m}$  observations. The CO (2 – 1) emission line has a size comparable to the [C II]  $158\mu\text{m}$  emission with an associated molecular gas mass of  $\approx 4.3 \times 10^{10} M_\odot$  (Shao et al. 2017). The [O III]  $88\mu\text{m}$  emission indicates a  $L[\text{O III}]/L_{\text{IR}}$  ratio comparable to local systems at similar  $L_{\text{IR}}$ . The quasar is luminous in X-ray as well and has a derived  $L_{2-10\text{keV}} = 6.93 \times 10^{44} \text{ erg s}^{-1}$  (Vito et al. 2019). In addition, there is evidence of companions close to the quasar although further confirmation is needed (D’Odorico et al. 2018; Feruglio et al. 2018). All together, J2310+1855 is an extraordinary quasar-starburst sample enabling us to study in detail a SMBH and galaxy co-evolution at  $z \sim 6$ .

In this paper, we present our new ALMA observations of CO (8 – 7), (9 – 8),  $\text{H}_2\text{O}(2_{0,2} - 1_{1,1})$  and  $\text{OH}^+(1_1 - 0_1)$  and NOEMA observation of CO (5 – 4), (6 – 5), (12 – 11) and (13 – 12) towards J2310+1855, aiming to investigate the molecular gas excitation mechanisms in environments of both intense star formation activity and luminous AGN. The paper is organized as follows: in Section 2 and 3, we present the observations and results. In Section 4, we analyze the CO SLED with a radiative transfer code to probe the physical conditions of molecular gas. In Section 5, we compare the CO excitation in J2310+1855 with local and high redshift galaxy samples and AGNs and discuss the heating mechanisms of molecular gas as well. Finally, we summarize the results in Section 6. We adopt a flat  $\Lambda\text{CDM}$

cosmology with  $H_0 = 70 \text{ km s}^{-1} \text{ Mpc}^{-1}$  and  $\Omega_m = 0.3$ , where  $1''$  corresponds to 5.7 kpc at the J2310 + 1855 redshift ( $z = 6.0031$ ), and the luminosity distance to J2310+1855 is 57763 Mpc.

## 2. OBSERVATIONS

### 2.1. ALMA

We observed the CO (8 – 7) ( $\nu_{\text{rest}} = 921.7997 \text{ GHz}$ ), CO (9 – 8) ( $\nu_{\text{rest}} = 1036.9124 \text{ GHz}$ ), H<sub>2</sub>O(2<sub>0,2</sub> – 1<sub>1,1</sub>) ( $\nu_{\text{rest}} = 987.9268 \text{ GHz}$ , hereafter H<sub>2</sub>O) and OH<sup>+</sup>(1<sub>1</sub> – 0<sub>1</sub>) ( $\nu_{\text{rest}} = 1033 \text{ GHz}$ , hereafter OH<sup>+</sup>) emission lines, as well as the underlying continuum towards  $z = 6.003$  quasar J2310+1855 with ALMA (Cycle 3, ID 2015.1.01265.S). All the observations were executed between April and November in 2016 with beam sizes between  $0''.6$  and  $0''.8$ . The CO (8 – 7), (9 – 8), H<sub>2</sub>O and OH<sup>+</sup> lines were observed in ALMA Band 4 with two separate executions, where 36 to 44 12-m diameter antennas were used during observations. For each observation, we used four spectral windows, each with a width of 1.875 GHz consisting of 128 channels, with two of the windows in the lower sideband (LSB) and the other two in the upper sideband (USB). The CO (8 – 7) and H<sub>2</sub>O lines were observed in one spectral setup, with one spectral window centered on the CO (8 – 7) observed frequency of 131.6274 GHz, one window covering the H<sub>2</sub>O emission, and the other two covering line-free dust continuum. In the other turning, we observed the CO (9 – 8) line centered at the frequency of 148.0648 GHz with the OH<sup>+</sup> line also covered in the same spectral window, while the other three windows measured the dust continuum. The fluxes were calibrated using the standard flux calibrator *Pallas*, while SDSS J2253+1608 was used as both the phase calibrator and the bandpass calibrator. The typical calibration uncertainty is  $< 5\%$  in ALMA band 4, here we use  $15\%$  uncertainty that also includes the uncertainties of the old *Pallas* flux model in early casa versions (Stanley et al. 2019).

The observational data were calibrated and reduced with the Common Astronomy Software Applications (CASA) software package version 4.7.0 (McMullin et al. 2007), using the standard ALMA pipeline. The maps were generated using the CLEAN task in CASA, and we apply the robust weighting algorithm with a Briggs parameter of 2 equivalent to natural weighting. This results in a FWHM synthesized beam size of  $0''.79 \times 0''.75$  and  $0''.77 \times 0''.63$  at CO (8 – 7)(H<sub>2</sub>O) and CO (9 – 8)(OH<sup>+</sup>) observing frequency, and  $0''.75 \times 0''.72$  and  $0''.80 \times 0''.65$  at 136.6 and 141.1 GHz for the continuum. The continuum level was determined using a first order polynomial, and the emission lines were imaged from the continuum subtracted data cube with all the line emitting channels included. With a total on source time of 34.9 and 30.3 minutes for CO (8 – 7)(H<sub>2</sub>O) and CO (9 – 8)(OH<sup>+</sup>), we finally binned the data of CO (8 – 7)(H<sub>2</sub>O) and CO (9 – 8)(OH<sup>+</sup>) to 36 and 32  $\text{km s}^{-1}$ , and the corresponding rms sensitivities were 0.17 and 0.19 mJy beam<sup>-1</sup> respectively. The sensitivity of the underlying continuum was  $15 \mu\text{Jy beam}^{-1}$ .

### 2.2. NOEMA

We observed CO (5 – 4) ( $\nu_{\text{rest}} = 576.2679 \text{ GHz}$ ), CO (6 – 5) ( $\nu_{\text{rest}} = 691.4731 \text{ GHz}$ ), CO (12 – 11) ( $\nu_{\text{rest}} = 1381.9951 \text{ GHz}$ ), CO (13 – 12) ( $\nu_{\text{rest}} = 1496.9229 \text{ GHz}$ ) and the underlying continuum of this quasar with NOEMA (Project W18EE). The CO (5 – 4) and (6 – 5) lines were observed in one tuning with the PolyFix correlator in Band 1 (3 mm), with the CO (5 – 4) line in the LSB and CO (6 – 5) in the USB, each with 7.744 GHz bandwidth. The observations were executed in A configuration on 2019 Jan 18 with a total observing time of 2 hours, with 1.18 hours on source while the rest of the time was expended for calibrations. A total number of 8 or 9 antennas were used. The CO (12 – 11) and (13 – 12) lines were observed in C/D configuration in Band 3 (1 mm) with one frequency setup, with the CO (12 – 11) line in the LSB and CO (13 – 12) in the USB, each with a 7.744 GHz bandwidth. The observations started on 2019 Apr 17 and ended on 2019 May 1. The total observing time was 8 hours with 6.2 hours on source, and a total number of 8 to 10 antennas were used in the observations. 3C454.3 was used as phase calibrator throughout all the CO observation. The typical calibration uncertainty is  $< 10\%$  in the 3 mm band and  $< 20\%$  in the 1 mm band.

The data were reduced with the Grenoble Image and Line Data Analysis System (GILDAS) software (Guilloteau & Lucas 2000) packages CLIC and MAPPING. We extracted the continuum from all line free channels in the  $uv$  plane with UV\_AVERAGE. The  $uv$  table of spectral lines was generated through UV\_SUBTRACT with the underlying continuum subtracted. Both the  $uv$  table of the continuum and spectral lines were cleaned with the HOGBOM algorithm and NATURAL weighting was used to ensure the maximum S/N. This results in a FWHM synthesized beam size of  $1''.67 \times 1''.37/1''.42 \times 1''.19$  for CO (5 – 4)/(6 – 5) and  $2''.08 \times 1''.62/1''.91 \times 1''.53$  for CO (12 – 11)/(13 – 12). The calibrated data of CO (5 – 4) and (6 – 5) were smoothed by a factor of 8 in frequency, resulting a spectral resolution of 16 MHz ( $\sim 60 \text{ km s}^{-1}$ ), and the calibrated CO (12 – 11) and (13 – 12) data were binned to 40 MHz ( $\sim 60 \text{ km s}^{-1}$ ) resolution.

The sensitivity was  $0.32 \text{ mJy beam}^{-1}$  for CO (5–4) and (6–5) and  $0.54 \text{ mJy beam}^{-1}$  for CO (12–11) and (13–12) per binned channels.

The observational details are listed in Table 1.

### 3. RESULTS

With ALMA, we detect the CO (8–7), (9–8) and H<sub>2</sub>O emission lines at  $25\sigma$ ,  $22\sigma$ , and  $15\sigma$ , respectively. The CO emission lines and the H<sub>2</sub>O line are marginally resolved. We also obtained a tentative signal ( $4\sigma$ ) for the OH<sup>+</sup> line on the red wing of the CO (9–8) line. The line intensity maps integrated over the line emitting channels are presented in Figure 1. The right panel of Figure 1 shows the line spectra integrated within the  $2\sigma$  contour in the intensity map. We calculate the line widths, redshift, and fluxes of CO (8–7), (9–8) and H<sub>2</sub>O by fitting a Gaussian profile to the spectra. We fit a 2D Gaussian component to the intensity maps of CO and H<sub>2</sub>O lines, and the source sizes are derived by deconvolving the fitted component with the beam. The spectral profiles of CO (9–8), (8–7) and H<sub>2</sub>O are similar (Figure 7), suggesting that the high  $J$  CO and H<sub>2</sub>O lines are probing similar regions. The source sizes measured from CO (9–8), (8–7) and H<sub>2</sub>O lines of  $\approx (0''.4 \pm 0''.1) \times (0''.3 \pm 0''.1)$  are slightly smaller than values found from previous CO (2–1) observation of  $(0''.6 \pm 0''.2) \times (0''.4 \pm 0''.2)$  and [C II]  $158\mu\text{m}$  observation of  $(0''.6 \pm 0''.1) \times (0''.4 \pm 0''.1)$  at similar spatial resolution (Wang et al. 2013; Feruglio et al. 2018; Shao et al. 2019). This may imply that CO (9–8), (8–7) and H<sub>2</sub>O lines trace similar dense molecular regions that are closer to the central SMBH compared to CO (2–1) and [C II]  $158\mu\text{m}$ . The redshift measured with the CO (9–8), (8–7), and H<sub>2</sub>O lines are within the uncertainties consistent with that from previous [C II], CO (2–1) and (6–5) observations (Wang et al. 2013; Feruglio et al. 2018; Shao et al. 2019). The OH<sup>+</sup> line is not as strong as the other detections, so we fix the center frequency to the [C II]  $158\mu\text{m}$  redshift, and fit a Gaussian profile to the spectra extracted from the peak pixel. As for the line widths, all the ALMA detections show line widths of  $\sim 400 \text{ km s}^{-1}$  consistent with previous CO and [C II] observations. From the OH<sup>+</sup> spectra, we find that there is an absorption like feature in the line center frequency, but the current S/N ratio is insufficient to confirm this feature. The continuum detection were published in Shao et al. (2019). The derived continuum source sizes of  $\approx (0''.30 \pm 0''.04) \times (0''.22 \pm 0''.06)$  are comparable to that measured with the CO and H<sub>2</sub>O lines.

We detected CO (5–4), (6–5), (12–11) and (13–12) with NOEMA. All of the four CO lines are unresolved. For the line widths, redshift, and fluxes calculation, we fit a Gaussian profile to the spectra extracted from the peak intensity pixel. The redshift measured with the CO (5–4), (6–5), (12–11) and (13–12) are consistent with our ALMA detections as well as previous CO and [C II] detections. The line width detected in ALMA and NOEMA observations are consistent. The CO (6–5) line has been previously detected with ALMA and the (pre-NOEMA) IRAM Plateau de Bure Interferometer (PdBI) with different spatial resolutions and the spectral line flux measured with ALMA is found to be only 70% of that found with the PdBI (Wang et al. 2013; Feruglio et al. 2018). In addition to the calibration uncertainties in different observations, it is also possible that the low resolution PdBI data include more flux from the extended region. The new NOEMA observation yield a CO (6–5) flux of  $1.05 \pm 0.07 \text{ Jy km s}^{-1}$ , consistent with the results obtained with ALMA (Feruglio et al. 2018). We also detected the underlying continuum at high S/N ratio. The measurements of redshift, line widths, line fluxes, and deconvolved source sizes of our ALMA and NOEMA observations as well as previous detections are summarized in Table 2, and the continuum measurements are listed in Table 3. The continuum, line intensity maps and spectra of CO (5–4), (6–5), (8–7), (9–8), (12–11), (13–12), H<sub>2</sub>O and OH<sup>+</sup> are shown in Figure 2 (NOEMA) and 1 (ALMA).

Figure 3 shows the velocity and velocity dispersion maps of [C II]  $158\mu\text{m}$  (Wang et al. 2013), CO (8–7), (9–8) and H<sub>2</sub>O. The velocity fields of CO (8–7), (9–8) and H<sub>2</sub>O overall follow the velocity gradient observed in [C II]  $158\mu\text{m}$  from north to south, which indicates that the emission might trace a rotating molecular gas disk. The velocity field of CO (8–7) shows a high velocity dispersion part in the western part, which is not observed in CO (9–8) and H<sub>2</sub>O. Such irregular velocity structure in CO (8–7) is likely to be a result of the low S/N. As for the velocity dispersion, CO (8–7), (9–8) and H<sub>2</sub>O show velocity dispersion of  $<100 \text{ km s}^{-1}$  in the outskirts (that is not likely influenced much by the beam smearing effect). Higher S/N observations, possibly at even higher angular resolution, are required in order to constrain the kinematic structures of the dense molecular gas.

### 4. RADIATIVE TRANSFER ANALYSIS OF THE CO SLED

In the CO SLED analysis, we also include a new detection of the CO (10-9) line from NOEMA at high S/N ratio. More details of the observation will be described in Riechers et al. (in prep). Our ALMA and NOEMA data, together

with previous detections of the CO (2 – 1) (Shao et al. 2019) and the CO (10 – 9) emission line, enable us to probe the the CO SLED of J2310+1855 from  $J = 2$  to  $J = 13$ , making it the most complete CO SLED ever obtained for a  $z \gtrsim 6$  quasar. We here use the radiative transfer model MOLPOP-CEP to investigate the physical conditions of the molecular gas, including the kinetic temperature  $T_{\text{kin}}$ , molecular hydrogen density  $n(\text{H}_2)$  and CO column density  $N(\text{CO})$ .

#### 4.1. Method

MOLPOP-CEP is a universal code that enables exact solutions of multi-level line emissions radiative transfer problems for all the atoms/molecules that have atomic/molecular data in the Leiden Atomic and Molecular Database (LAMDA) database (Elitzur & Asensio Ramos 2006; Asensio Ramos & Elitzur 2018). This code assumes a slab geometry with the emitting region divided into several zones and treats the radiative transfer problem with a coupled escape probability (CEP) method that aims to solve the coupled level population equations of different zones under consideration. Dividing the geometry into several zones makes it possible to solve the level populations as a function of depth into the line emitting region and also leads to more accurate solutions compared to previous large velocity gradient (LVG) models.

The physical parameters as inputs control the number of zones that the geometry is divided and the physical parameters of the individual zone in the slab geometry. Even for a uniform physical parameter setup in the whole geometry, the division of geometry into zones is necessary to increase the accuracy of the results. This is because, for optically thick lines, the strength of radiative reactions changes with distances to the surface, and the transition level population distributions depend on positions in the geometry (Asensio Ramos & Elitzur 2018). In the slab, each zone in principle can have different physical parameter setups including: (1) the zone width  $\Delta L$ , (2) the gas density within the zone  $n(\text{H}_2)$ , (3) kinetic temperature  $T_{\text{kin}}$ , (4) molecular abundance, (5) local linewidth (which corresponds to the line absorption/emission profile in each point in the geometry). Besides these, MOLPOP-CEP allows the inclusion of external radiation field. Given these physical parameters, the code will then solve the coupled level population problem between zones and finally predict the emergent intensities of the emission lines that can be directly compared to the observations. We assume uniform parameters for each slab. The accuracy of MOLPOP-CEP solutions increases with the number of zones. Here we divide the geometry into 10 zones for the model calculation as is suggested by Asensio Ramos & Elitzur (2018).

We generate a grid of slab models through varying the physical parameters of greatest interest – the gas density  $n(\text{H}_2)$ , temperature  $T_{\text{kin}}$  and zone width  $\Delta L$ . For the other two zone parameters, we fix the molecular abundance of CO to  $X_{\text{CO}} = 10^{-4}$  (Milky Way, Blake et al. 1987), and local linewidth to  $1 \text{ km s}^{-1}$  for all the model calculations. In addition, we include the CMB at the quasar redshift of 19.12 K, because the hot CMB at high redshift will 1) acts as an extra heating source of the CO emission, 2) serves as a continuum background (Da Cunha et al. 2013; Zhang et al. 2016). In each model, all of the 10 zones have the same physical parameter setup thus each model in the grid can be described by a uniform  $n(\text{H}_2)$ ,  $T_{\text{kin}}$  and  $\Delta L$ . The CO column density within the geometry, which is the sum of the column densities of 10 zones, is proportional to the zone width  $\Delta L$  through:

$$N(\text{CO}) = 10 \times n(\text{H}_2) \times \Delta L \times X_{\text{CO}}. \quad (1)$$

In the rest of the paper, we use  $n(\text{H}_2)$ ,  $T_{\text{kin}}$  and  $N(\text{CO})$  to characterize the physical condition of each slab grid. As it is easier to use  $N(\text{CO})$  rather than  $\Delta L$  to make comparisons with constraints from observations (see section 4.2). The final grid covers the typical physical conditions of the molecular clouds with a temperature range of 20 – 800 K, density of  $10^3 - 10^8 \text{ cm}^{-3}$  and CO column density of  $10^{14} - 10^{21} \text{ cm}^{-2}$  (this corresponds to  $\text{H}_2$  column density of  $10^{18} - 10^{25} \text{ cm}^{-2}$  for our assumed  $X_{\text{CO}}$  of  $10^{-4}$ ). More details about the grid are listed in Table 4.

We use the model grid to fit our observed CO SLED of J2310+1855. The fitting procedure is as follows: we first apply the least square method to find the best fitting results. We also use the Bayesian code emcee (Foreman-Mackey et al. 2013) to efficiently explore the parameter space and get the posterior probability distributions of all the parameters considered. Emcee is an extensible, pure-Python implementation that is designed for Bayesian parameter estimation using Ensemble samplers with affine invariance (Goodman & Weare 2010).

#### 4.2. Parameter Constraints

During the fitting procedure, we set constraints for the three parameters:  $T_{\text{kin}}$ ,  $n(\text{H}_2)$  and  $N(\text{CO})$ . The fact that  $T_{\text{kin}}$  is hotter than the background CMB radiation at redshift 6 is a prior, which sets  $T_{\text{kin}} > 19.12 \text{ K}$ . As for column

density, one prior is that the total amount of gas producing the observed CO luminosities should be no more than the total dynamical mass of this system, this leads to:

$$N(\text{CO})\Phi_A < \frac{M_{\text{dyn}}X_{\text{CO}}}{\mu m_{\text{H}_2}A} [\text{cm}^{-2}], \quad (2)$$

where  $\Phi_A$  is the filling factor,  $M_{\text{dyn}}$  is the dynamic mass,  $A$  is the source area in  $\text{cm}^2$ ,  $\Delta V$  is the CO line width in  $\text{km s}^{-1}$ ,  $\mu$  is the mean molecular weight,  $m_{\text{H}_2}$  is the  $\text{H}_2$  molecule mass and  $X_{\text{CO}}$  is the CO abundance. The source size and gas dynamical mass are adopted from [Shao et al. \(2019\)](#), with  $M_{\text{dyn}} \approx 4.3 \times 10^{10} M_{\odot}$  and  $A \approx \frac{\pi}{4} \times 0.60 \times 0.40 \text{ arcsec}^2$ . Adopting a CO to  $\text{H}_2$  abundance ratio  $X_{\text{CO}} = 10^{-4}$ , and  $\mu = 1.4$  for mean molecular weight, the final constraint is:

$$N(\text{CO})\Phi_A < 3.2 \times 10^{19} [\text{cm}^{-2}]. \quad (3)$$

The other prior for column density is that it should be less than the source gas volume density integrated along line of sight for line emitting regions. This leads to:

$$N(\text{CO}) < n(\text{H}_2) \times X_{\text{CO}} \times S [\text{cm}^{-2}], \quad (4)$$

where  $S$  is the source size along the line of sight,  $n(\text{H}_2)$  is the  $\text{H}_2$  volume density. Assuming a largest diameter of CO emitting region of  $0''.60$  ([Shao et al. 2019](#)), we set a constraint on both  $N(\text{CO})$  and  $n(\text{H}_2)$  as follows:

$$\frac{N(\text{CO})}{n(\text{H}_2)} < 1.1 \times 10^{18} [\text{cm}]. \quad (5)$$

#### 4.3. Fitting Results

We endeavor to probe the physical conditions of the molecular gas in J2310+1855 by fitting a one-component model to the CO SLED. Calibration uncertainties are included in all the modeling processes throughout the paper. We first fit the grid models to the observed CO SLED with the least square method. The left panel of Figure 4 shows the best fitting result, suggesting a “warm” and “dense” gas component with kinetic temperature of  $T_{\text{kin}} = 228$  K, density of  $\log(n(\text{H}_2)/\text{cm}^{-3}) = 4.75$  and column density of  $\log(N(\text{CO})/\text{cm}^{-2}) = 17.5$ . We then search for all the possible physical conditions that fit the observational CO SLED with the emcee code. The posterior probability distributions of the three parameters are shown in Figure 5. This indicate that the data can be fitted with a “warm” and “dense” gas component with parameter range of  $T_{\text{kin}} \approx 167_{-56}^{+153}$  K,  $\log(n(\text{H}_2)/\text{cm}^{-3}) \approx 5.11_{-0.58}^{+1.83}$  and  $\log(N(\text{CO})/\text{cm}^{-2}) \approx 17.28_{-0.42}^{+0.33}$ .<sup>1</sup> But the current best fit model fail to reproduce the very high CO (8 – 7) line flux detected.

Previous CO SLED modeling from local to high redshift galaxies/AGNs suggest different gas physical properties in different systems. E.g., in the  $z = 2.56$  quasar cloverleaf ([Riechers et al. 2011](#)) and the  $z = 6.34$  starburst galaxy HLFS3 ([Riechers et al. 2013](#)), a single gas component is able to reproduce the observed CO SLED. In addition, more than one gas component is found in the CO SLED analysis of local starburst galaxies, (U)LIRGs, and even the quasars at the highest redshift (e.g., M82, NGC 1068, Mrk 231, APM 08279+5255, J0100+2802, J0439+1634 and J1148+5251 ([Weiß et al. 2005, 2007](#); [Panuzzo et al. 2010](#); [van der Werf et al. 2010](#); [Spinoglio et al. 2012](#); [Gallerani et al. 2014](#); [Wang et al. 2019](#); [Yang et al. 2019](#))). The CO SLED of the  $z = 6.3$  quasar J0100+2802 suggests two components of gas with a “cold” component with  $T_{\text{kin}} \approx 24$  K,  $\log(n(\text{H}_2)/\text{cm}^{-3}) \approx 4.5$  and a “warm” component with  $T_{\text{kin}} \approx 224$  K,  $\log(n(\text{H}_2)/\text{cm}^{-3}) \approx 3.6$  ([Wang et al. 2019](#)). The CO SLED of J0439+1634 at  $z = 6.5$  indicates a “cold” component with  $T_{\text{kin}} \approx 23$  K and  $\log(n(\text{H}_2)/\text{cm}^{-3}) \approx 4.1$  in combination with a “warm” component with  $T_{\text{kin}} \approx 140$  K and  $\log(n(\text{H}_2)/\text{cm}^{-3}) \approx 4.5$  ([Yang et al. 2019](#)). The cold component was thought to be associated with the submm/mm-detected dust component powered by active star formation with temperatures of  $40 \sim 60$  K (assuming optically thin, [Beelen et al. 2006](#); [Leipski et al. 2013](#)). The dust continuum SED fitting of J2310+1855 indicates a dust temperature of  $\sim 40$  K in the optically thin dust assumption of [Shao et al. \(2019\)](#) or 76 K in the optically thick assumption of [Carniani et al. \(2019\)](#). Both are much lower than the one-component fitting result of  $T_{\text{kin}} = 228$  K. As the one-component best-fit model fails to explain the observed CO (8-7) flux (left panel of Figure 4), it is possible that there is an additional “cold” gas component physically associated with the submm/mm detected dust in J2310+1855. Motivated by the above, we examine whether the data can be explained with a two-component model.

<sup>1</sup> The resulting parameter ranges are consistent within  $1\sigma$  between including and excluding the CO (10 – 9) line in the fitting procedure.

The two-component model fitting to the data requires eight parameters, including the physical parameters ( $T_{\text{kin}}$ ,  $n(\text{H}_2)$  and  $N(\text{CO})$ ) and the normalization of each component. Our data are insufficient to constrain all eight parameters. Considering that the “cold” component is usually physically connected to and has similar temperature as that of the cold dust (as is explained in detail in the previous paragraph), and the dust temperature of J2310+1855 is not well constrained ( $T_{\text{dust}}$  ranges between 40 – 80 K depending on the dust model assumed), we will fix the “cold” component to the typical “cold” gas physical conditions observed in  $z \sim 6$  quasar in the following analysis. With this assumption, we are fitting only five instead of eight parameters. As a consequence, the model parameters could be better constrained. We adopt a typical “cold” gas component with physical parameters of  $T_{\text{kin}} \approx 50$  K and  $\log(n(\text{H}_2)/\text{cm}^{-3}) = 4.2$  that is observed in a “typical”  $z \sim 6$  quasar J1148+5251 (Riechers et al. 2009). Because column density is not one of the model parameters in Riechers et al. (2009), we use a column density of  $\log(N(\text{CO})/\text{cm}^{-2}) = 18.0$  for the “cold” model. We note that the resulting  $X_{\text{CO}}/dv/dr$  here is different from that in Riechers et al. (2009), because in the MOLPOP-CEP model, the  $dv/dr$  is derived from the first principle and is different in different places in the whole geometry. The final “cold” model using the set of parameters we adopted here can well represent the observational CO SLED of J1148+5251 presented in Riechers et al. (2009). The right panel of Figure 4 shows the minimum  $\chi^2$  fitting result of the two-components model. The resulting “warm” component with the minimum  $\chi^2$  has a physical condition of  $T_{\text{kin}} = 306$  K,  $\log(n(\text{H}_2)/\text{cm}^{-3}) = 5.25$  and  $\log(N(\text{CO})/\text{cm}^{-2}) = 15.5$ . We find in the fitting result that the “cold” component (the J1148+5251 model) dominates the low  $J$  ( $J = 2$ ) part, and contributes to 77% of the observed CO (2 – 1) flux. As we have already mentioned before, the low  $J$  CO emission lines trace the total molecular gas mass, thus the “cold” component dominates the total molecular gas mass. In the mid- $J$  ( $J = 5, 6$ ) part, the contribution of the “cold” component decreases and only accounts for  $\sim 30\%$  of the observed CO fluxes. And in the high  $J$  ( $J \geq 8$ ) part, the “cold” component contribution is negligible. The “warm” component, that barely contributes to the total molecular gas mass, dominates the CO SLED from the mid- to the high- $J$  ( $J \geq 5$ ) part of the overall CO SLED. The posterior probability distributions of the parameters calculated by the emcee code are shown in Figure 5. It suggest a “warm” and “dense” component with parameter range of  $T_{\text{kin}} \approx 306_{-149}^{+263}$  K,  $\log(n(\text{H}_2)/\text{cm}^{-3}) \approx 5.22_{-0.49}^{+1.04}$  and  $\log(N(\text{CO})/\text{cm}^{-2}) \approx 15.29_{-1.17}^{+1.34}$ .<sup>2</sup>

To summarize, the best one-component “warm” and “dense” model reproduces the observed CO SLED in general, except for an underestimation of the CO (8 – 7) flux. The two-component fitting result suggests the CO SLED at  $J \geq 5$  is dominated by a “warm” and “dense” gas component, while the “cold” component barely contribute to the mid- to the high- $J$  CO fluxes but dominate the total molecular gas mass. Either one or two component model suggests that the CO SLED detected within the nuclear region (source size of  $\sim 2$  kpc) of the quasar host is dominated by a “warm” and “dense” gas component at  $J \geq 5$ .

## 5. DISCUSSION

### 5.1. The CO emission in J2310+1855 compared with local starburst systems

The CO SLED reveals the physical conditions of molecular gas (e.g., the illuminating radiation field strength, kinetic temperature, volume density and column density). We first compare the CO SLED of J2310+1855 with local starburst systems. Figure 6 (a) shows the CO SLED of J2310+1855 compared with two local starburst samples. They are local (U)LIRGs sample consisting of 29 (U)LIRGs (Rosenberg et al. 2015) and local normal + starburst galaxy sample consisting of 43 star-forming galaxies (SFGs) and 124 (U)LIRGs (Liu et al. 2015). Although there are actually a small number of AGNs contained in the two (U)LIRGs comparison samples, they are confirmed to impact negligibly on both the CO flux and the infrared luminosity (Rosenberg et al. 2015). For the Rosenberg et al. (2015) sample, we exclude NGC 6240 in sample mean calculation (because this AGN represents a very extreme CO SLED, see details in Section 5.2). Through comparisons, we find that the peak of CO SLED is  $\lesssim 4$  for all the local starburst samples, while the J2310+1855 CO SLED peaks at much higher  $J$  transitions at  $J = 8$ . The CO emission lines of J2310+1855 show higher excitation compared to all local (U)LIRG samples (i.e., the CO flux is higher than the average of all the local ULIRG samples and is also well above the range of all the comparison samples especially for  $J \geq 8$ ). In addition, we compare J2310+1855 with a representative example of local starburst galaxy M82 in Figure 6 (b). We get a similar result as that of the starburst samples. The CO SLED of M82 peaks at  $J = 5$  and decreases dramatically at  $J \geq 8$ , contrary to J2310+1855 that peaks at  $J = 8$  and is luminous even at  $J \geq 10$ .

<sup>2</sup> The resulting parameter ranges are consistent within  $1\sigma$  between including and excluding the CO (10 – 9) line in the fitting procedure.

The high CO excitation detected in the J2310+1855 nuclear region (source size of  $\sim 2$  kpc in FWHM) may indicate other heating mechanisms besides the UV heating from massive young stars (e.g., mechanical heating by shocks, X-ray heating from AGNs), or very intense UV radiation field (e.g., large UV photon flux produced by a result of both the quasar and the star formation, see Section 5.5 for further discussions about these heating mechanisms).

### 5.2. The CO emission in J2310+1855 compared with local AGNs

We compare the CO emission lines of J2310+1855 with some representative local AGNs (Mrk 231, NGC 1068 and NGC 6240). The AGNs we selected are thoroughly studied local AGNs that represent different CO heating mechanisms. NGC 1068 is one of the closest AGN, whose high  $J$  CO emission lines in the circumnuclear disk (CND) are best explained by a XDR model, and the starburst ring at larger radii that dominates the molecular gas mass is best fitted with a PDR model (Spinoglio et al. 2012). Mrk 231 requires an XDR model to fit the high  $J$  CO emission lines in the central 160 pc molecular region, although the low  $J$  CO lines are mainly from the PDR component at larger distances (van der Werf et al. 2010). NGC 6240 is a local AGN with three nucleus, the CO emission lines are unlikely to correlate with the position of either AGN nuclei and mechanical heating is proposed to interpret the extremely excited CO SLED and also the optical ISM emission lines (Meijerink et al. 2013; Kollatschny et al. 2019).

Figure 6 (b) shows the CO SLED of J2310+1855 and the local AGNs. The CO SLED of NGC 1068 peaks at  $J \leq 4$ , and then decreases rapidly with increasing  $J$ . Mrk 231 shows an extreme CO SLED that peaks at  $J = 5$  and displays a high normalized CO flux even at  $J \approx 10 - 13$ . The differences between NGC 1068 and Mrk 231 can be explained by different X-ray energy input to the CO heating, evident from the higher X-ray flux derived in Mrk 231 ( $28 \text{ erg cm}^{-2} \text{ s}^{-1}$ , van der Werf et al. 2010) than NGC 1068 ( $9 \text{ erg cm}^{-2} \text{ s}^{-1}$ , Spinoglio et al. 2012). NGC 6240 shows the most extreme CO SLED among these three AGNs. The quasar J2310+1855 peaks at higher  $J$  ( $J = 8$ ) compared to these local AGNs, i.e., the gas in the nuclear region of J2310+1855 has higher excitation compared to that of the local AGNs.

### 5.3. The CO emission in J2310+1855 compared with high redshift systems

We also compare the CO SLED of J2310+1855 with high redshift systems, including high redshift (lensed) SMGs and quasars. Figure 6 (a) shows the CO SLED of J2310+1855 and high redshift SMGs: a sample of  $z \sim 1.2 - 4.1$  SMGs (Bothwell et al. 2013) and a sample of  $15 z \sim 2 - 4$  lensed SMGs from Carilli & Walter (2013) and Yang et al. (2017). The high redshift SMG CO SLEDs peak at  $J \lesssim 6$ , while J2310+1855 peaks at higher  $J$  ( $J = 8$ ) than the two SMG samples. This is similar to the results when comparing the J2310+1855 CO SLED to local starburst samples.

We also select some well-known high redshift quasars for comparison. Including two lensed quasars, the Cloverleaf at  $z = 2.56$  and APM 08279+5255 at  $z = 3.91$ . The fit to the CO SLED detected in the very central region of APM 08279+5255 requires an XDR component dominating the high  $J$  CO emission lines (Bradford et al. 2011). We also include three  $z \gtrsim 6$  quasars that are detected in at least 4 CO transitions: J1148+5251, J0439+1634, and J0100+2802 (Bertoldi et al. 2003; Walter et al. 2003; Beelen et al. 2006; Riechers et al. 2009; Gallerani et al. 2014; Wang et al. 2019; Yang et al. 2019). Together with J2310+1855, this allows us to do a systematic study of the CO emission lines in the quasar-starburst systems at the highest redshift. Figure 6 (c) shows the CO SLED of J2310+1855 compared to other high redshift quasars. APM 08279+5255 exhibits the most extreme CO SLED that is detected in the nuclear 550 pc size scale, and it represents a highly excited nuclear CO SLED exposed to the intense X-rays from the quasar. The limited CO detections in J0439+1634 and Cloverleaf suggests that maybe the CO SLED peaks at  $J = 8 \sim 10$  similar to J2310+1855. As for J1148+5251 and J0100+2802, we are not able to determine the CO SLED peak. This is because for J0100+2802, there is no CO observation at  $J = 8, 9$  and  $J > 11$ , while the CO SLED of J1148+5251 is observed at  $J \leq 7$  and  $J = 17$ . The comparison of CO SLEDs between J2310+1855 and other high- $z$  quasars suggest that a highly excited molecular gas component is common in the nuclear region of the quasar hosts. However, as described above, the shape of the CO SLED of these systems are different from object to object. Due to the lensing effect, the CO SLED of APM 08279+5255 may represent molecular gas on  $< 1$  kpc scale. The CO SLED of J2310+1855 is not as extreme as APM 08279+5255, and more comparable to the Cloverleaf. When compared to the two  $z > 6$  quasars, J0100+2802 and J0439+1634, that have available CO data at  $J = 8 \sim 11$ , J2310+1855 is more single-peaked no flatten or turn over around  $J = 6$ . It is possible that the cold star forming component contribute more to the flux of the mid- $J$  CO in the cases of J0100+2802 and J0439+1634.

### 5.4. $H_2O$ and $OH^+$ emission

Recent studies found linear relations between the infrared luminosity and the  $\text{H}_2\text{O}(2_{0,2} - 1_{1,1})$  luminosity in local and high redshift infrared bright systems, suggesting the excitation of this water transition is dominated by infrared pumping (van der Werf et al. 2011; Yang et al. 2016; Jarugula et al. 2019). We first compare the  $\text{H}_2\text{O}$  detection of J2310+1855 to the local and high redshift (U)LIRGs. Figure 7 shows the  $L_{\text{H}_2\text{O}}$  and  $L_{\text{IR}}$  for local and high redshift (U/Hy)LIRGs and AGNs. The black dashed line is the best fit to the local and high redshift (U/Hy)LIRGs presented in Figure 3 of Yang et al. (2016). We consider the infrared luminosity of J2310+1855 in two cases: 1) we adopt total infrared luminosity from both the quasar and the host galaxy ( $L_{\text{IR}(\text{total})}$ ); 2) we use the infrared luminosity only from the host galaxy ( $L_{\text{IR}(\text{galaxy})}$ , Shao et al. 2019). The linear relation is fitted with (U/Hy)LIRGs (local and high  $z$ ) and dusty star-forming galaxies, while all the four plotted AGNs including J2310+1855 are well below this relation. This is because the AGNs not only provide the power source of water emission but also contribute significantly to the infrared luminosity (van der Werf et al. 2011; González-Alfonso et al. 2010). As for the host galaxy infrared luminosity case, J2310+1855 reveals a slightly higher water luminosity given its galaxy IR luminosity compared to the linear relation. The velocity dispersion map of the  $\text{H}_2\text{O}$  shows a velocity dispersion of  $<100 \text{ km s}^{-1}$ , suggesting that it may not be the large velocity dispersion that contributes to the luminous water emission. Higher spatial resolution observations are required to confirm this. We find in J2310+1855 slightly higher  $L_{\text{H}_2\text{O}}/L_{\text{IR}}$  ratio than that for local and high redshift (U/Hy)LIRGs. At  $z \sim 6$ , only a few quasars are detected in water emission (Bañados et al. 2015; Yang et al. 2019). Similar result is found in the  $z = 6.52$  quasar J0439+1634, where a higher  $L_{\text{H}_2\text{O}(3_{2,1}-3_{1,2})}/L_{\text{IR}}$  ratio is found as compared to the linear relation (Yang et al. 2019).

To further investigate the heating sources of molecular gas, we also study the ratio between  $\text{H}_2\text{O}$  and CO in J2310+1855. Extremely luminous  $\text{H}_2\text{O}$  emission is not expected in typical PDRs. E.g., in the Orion bar (a representative dense PDR with  $n \sim 10^5 \text{ cm}^{-3}$  illuminated by an intense FUV radiation field of  $G_0 = 4 \times 10^4$ ), the  $L_{\text{H}_2\text{O}}/L_{\text{CO}(6-5)}$  ratio is 0.20 (Habart et al. 2010; Putaud et al. 2019). Another example is the local starburst galaxy M82 that shows a ratio of 0.06 (Kamenetzky et al. 2012). If the physical/chemical condition is dominated by shocks or X-rays, then the  $L_{\text{H}_2\text{O}}/L_{\text{CO}(6-5)}$  ratio can be even as high as unity. NGC 1266 is an S0 galaxy highly excited in molecular gas, and Pellegrini et al. (2013) found a  $L_{\text{H}_2\text{O}}/L_{\text{CO}(6-5)}$  ratio of 0.96 that can be only explained by shocks. Mrk 231 is a representative of the molecular gas heated by X-rays, and it has a  $L_{\text{H}_2\text{O}}/L_{\text{CO}(6-5)}$  ratio of  $1.10 \pm 0.17$  (González-Alfonso et al. 2010). The quasar J2310+1855 exhibits a  $L_{\text{H}_2\text{O}}/L_{\text{CO}(6-5)}$  ratio of  $0.97 \pm 0.09$ , which is comparable to Mrk 231 and NGC 1266 but is much higher than Orion bar and M82. These suggest that the molecular gas heating is not likely dominated by PDR. In addition, we also consider the high redshift lensed SMGs for comparison (Omont et al. 2013; Yang et al. 2013, 2016, 2017). These lensed SMGs are all starbursts that are exposed to intense radiation field and shocks, and some have extremely luminous water emission lines that can not be purely explained by PDR. For the majority of the SMGs, the  $L_{\text{H}_2\text{O}}/L_{\text{CO}(6-5)}$  ratio is found to be less than 0.8, while only quite a few objects have ratios of  $\sim 1$  that is unlikely PDR. The even higher  $L_{\text{H}_2\text{O}}/L_{\text{CO}(6-5)}$  ratio of J2310+1855 compared to typical high redshift lensed SMGs might suggest additional gas heating by the central luminous quasar. We also compare the  $\text{H}_2\text{O}/\text{CO}$  ratio of the quasar with other  $z \sim 6$  quasars that are detected in water emission. J0439+1634 was detected in the  $\text{H}_2\text{O}(3_{2,1} - 3_{1,2})$  emission, and suggest a  $L_{\text{H}_2\text{O}(3_{2,1}-3_{1,2})}/L_{\text{CO}(6-5)}$  ratio of  $1.23 \pm 0.22$ . Adopting a mean  $\text{H}_2\text{O}(3_{2,1}-3_{1,2})/\text{H}_2\text{O}(2_{0,2}-1_{1,1})$  of 1.4 estimated from SMGs in Yang et al. (2016), we estimate the  $L_{\text{H}_2\text{O}}/L_{\text{CO}(6-5)}$  ratio in J0439+1634 of  $0.86 \pm 0.17$ , which is comparable to the value of J2310+1855.

We tentatively detected the  $\text{OH}^+$  line at a S/N of 4. The spectra of the  $\text{OH}^+$  line shows a P Cygni like profile, with a possible absorption in the line center frequency. This might hint on possible outflows/inflows in this source, although further high sensitivity observations are needed to confirm this. The ratios between  $\text{OH}^+$ ,  $\text{H}_2\text{O}^+$  and  $\text{H}_3\text{O}^+$  reactive molecular ions are ideal tracers of the ionization rate and serve as the ionization source diagnostics. In J2310+1855, we are not able to constrain the ionization rate with the  $\text{OH}^+$  detection alone. On the other hand,  $\text{OH}^+$  and  $\text{H}_2\text{O}$  are all oxygen-hydrogen species, and  $\text{OH}^+$  can be formed by photodissociation of  $\text{H}_2\text{O}$ , accordingly we are expecting higher  $L_{\text{OH}^+}/L_{\text{H}_2\text{O}}$  ratio in the presence of cosmic rays or X-rays. Mrk 231 is one of the best studied AGNs that has been detected in a series of  $\text{OH}^+$ ,  $\text{H}_2\text{O}^+$  and  $\text{H}_3\text{O}^+$  emission lines. González-Alfonso et al. (2018) detected very bright  $\text{OH}^+$  emission with  $L_{\text{OH}^+}/L_{\text{H}_2\text{O}}$  ratio of  $0.37 \pm 0.13$ . The ionization rate derived by making use of all the molecular ions detected are very high, and even can not be explained by its observed X-ray flux and requires ionization by cosmic rays (i.e., the ionization rate produced by X-ray photons is  $\sim 1/10$  the value required). The quasar J2310+1855 exhibit a  $L_{\text{OH}^+}/L_{\text{H}_2\text{O}}$  ratio of  $0.20 \pm 0.15$  comparable with Mrk 231. The observed X-ray luminosity in J2310+1855 is  $\sim 170\times$  that observed in Mrk 231 (Vito et al. 2019). If we simply assume similar ionization rate in J2310+1855 as that of Mrk

231 (as the  $L_{\text{OH}^+}/L_{\text{H}_2\text{O}}$  ratios are comparable in these two AGNs), the X-ray photons from J2310+1855 are more than adequate to explain the observed  $\text{OH}^+$  emission.

### 5.5. Molecular gas heating mechanisms

In the CO SLED modeling of J2310+1855, we find the mid to high  $J$  ( $J \geq 5$ ) CO emission lines are dominated by a “warm” and “dense” gas component with  $T \gtrsim 150$  K,  $\log(n(\text{H}_2)/\text{cm}^{-3}) \gtrsim 5$  and  $\log(N(\text{CO})/\text{cm}^{-2}) \gtrsim 15.0$ . Such “warm” and “dense” gas component is warmer and denser than typical values found in local (U)LIRGs (Papadopoulos et al. 2012, 2013), and comparable to the extreme cases, e.g., the NGC 1068 circumnuclear disk (Krips et al. 2011; Viti et al. 2014), and highly excited (U)LIRGs (Papadopoulos et al. 2012, 2013). Studies of local and high redshift systems suggest that the molecular gas can be heated through 1) the UV heating from young massive stars or AGNs, 2) mechanical heating by shocks generated from supernovae or AGN outflows, 3) cosmic ray heating from supernovae or AGNs, or 4) X-ray heating from the AGNs (Bradford et al. 2003; Bradford et al. 2011; Spinoglio et al. 2012; Meijerink et al. 2013; Rosenberg et al. 2015; Uzgil et al. 2016). We inspect the most possible mechanism that contributes to the high CO excitation and luminous  $\text{H}_2\text{O}$  and  $\text{OH}^+$  emission lines observed in J2310+1855.

To investigate the PDR origin, we fit the CO SLED of J2310+1855 to the PDR grid (Meijerink et al. 2007), and the best fitting result indicates a FUV flux of  $G_0 = 1.0 \times 10^4$  and  $n \sim 5.6 \times 10^5 \text{ cm}^{-3}$ . This suggests a higher FUV flux than that reported in Carniani et al. (2019) due to the lack of information from the  $J \geq 10$  CO lines in their study. Although the CO emission can be explained by a dense PDR illuminated by an intense FUV radiation field, the bright  $\text{H}_2\text{O}$  and  $\text{OH}^+$  emission lines (high  $\text{H}_2\text{O}/\text{CO}$  and  $\text{OH}^+/\text{H}_2\text{O}$  ratio) hint at different physical and chemical conditions than in a PDR, suggesting rather the presence of X-rays, shocks or cosmic rays that heat and ionize the molecular gas. In the nuclear region, both the star formation activity and the luminous quasar are capable of influencing the physical and chemical conditions of the molecular gas. The powerful quasar is able to participate in all the possible gas heating mechanisms through the X-ray it radiates, the shocks generated by AGN outflows and the cosmic rays it produces.

## 6. SUMMARY

We report new detections of CO (5 – 4), (6 – 5), (12 – 11) and (13 – 12) with NOEMA and CO (8 – 7), (9 – 8),  $\text{H}_2\text{O}$  and  $\text{OH}^+$  with ALMA in the  $z = 6.003$  quasar J2310+1855. This is the most complete SLED ever obtained for a  $z \geq 6$  quasar. We spatially resolved the CO (8 – 7), (9 – 8) and  $\text{H}_2\text{O}$  lines at similar source sizes of  $\sim 2$  kpc in FWHM, which are slightly more compact than the [C II]  $158\mu\text{m}$  and CO (2 – 1) emission lines. These suggest that the high  $J$  CO lines and the  $\text{H}_2\text{O}$  line are probing the nuclear dense molecular regions closer to the quasar. We analyze the physical conditions of the molecular gas through CO SLED modeling and we also compare the CO emission lines from the quasar with local and high redshift starburst samples and some representative local and high redshift AGNs. The main results are summarized below.

- The CO SLED of J2310+1855 at  $J \geq 5$  is dominated by a “warm” and “dense” gas component in the parameter range of  $T_{\text{kin}} \approx 167_{-56}^{+153}$  K,  $\log(n(\text{H}_2)/\text{cm}^{-3}) \approx 5.11_{-0.58}^{+1.83}$  and  $\log(N(\text{CO})/\text{cm}^{-2}) \approx 17.28_{-0.42}^{+0.33}$  (in the one-component model) or  $T_{\text{kin}} \approx 306_{-149}^{+263}$  K,  $\log(n(\text{H}_2)/\text{cm}^{-3}) \approx 5.22_{-0.49}^{+1.04}$  and  $\log(N(\text{CO})/\text{cm}^{-2}) \approx 15.29_{-1.17}^{+1.34}$  (in the two-component model). We are not able to rule out a “cold” component that dominates the molecular gas mass but barely contributes to the  $J \geq 5$  CO fluxes.

- The CO SLED of J2310+1855 shows higher excitation compared to local/high redshift starburst samples and local AGNs. Such high CO excitation is also found in other  $z \gtrsim 6$  quasars (e.g., J1148+5251, J0100+2802, J0439+1634), and lensed high redshift quasars (e.g., APM 08279+5255, the Cloverleaf).

- The  $L_{\text{H}_2\text{O}}/L_{\text{IR}(\text{galaxy})}$  ratio in this quasar is higher than local and high  $z$  (U/Hy)LIRGs. The luminous detections of  $\text{H}_2\text{O}$  and  $\text{OH}^+$  (high  $\text{H}_2\text{O}/\text{CO}$  and  $\text{OH}^+/\text{H}_2\text{O}$  ratios) are suggesting other heating and ionization sources (e.g., cosmic rays, shocks and X-rays) in addition to PDR. In the nuclear region, the luminous quasar and the starburst activity are able to impact on the molecular gas through all these possible mechanisms.

Complete measurements of the CO SLED of the quasar hosts at  $z \geq 6$  are of great importance for our understanding of the physical conditions and the heating mechanisms of the molecular gas in the complex environment with both AGN and nuclear starburst activities. It is also essential for the higher resolution observations to map the distributions and kinematics of the highly excited molecular gas around the AGN.

**Table 1.** Observational Details

Line ID	$\nu_{\text{obs}}$	$\delta\nu(\delta v)$	Band	$T_{\text{source}}$	$T_{\text{tot}}$	rms
	GHz	MHz (km s <sup>-1</sup> )		mins	mins	mJy beam <sup>-1</sup>
(1)	(2)	(3)	(4)	(5)	(6)	(7)
CO (5 – 4)	82.2875	16(58)	NOEMA 3 mm	70.8	120	0.32
CO (6 – 5)	98.7381	16(49)	-	-	-	-
CO (8 – 7)	131.6274	15.625(36)	ALMA Band 4	34.9	53.3	0.17
H <sub>2</sub> O(2 <sub>0,2</sub> – 1 <sub>1,1</sub> )	141.0699	15.625(36)	-	-	-	-
CO (9 – 8)	148.0648	15.625(32)	ALMA Band 4	30.3	48.5	0.19
OH <sup>+</sup> (1 <sub>1</sub> – 0 <sub>1</sub> )	147.5061	15.625(32)	-	-	-	-
CO (12 – 11)	197.3405	40(61)	NOEMA 1 mm	372	600	0.54
CO (13 – 12)	213.7515	40(56)	-	-	-	-

NOTE—Column 1: Line ID; Column 2: Line center frequency in the observer frame; Column 3: Binned spectral resolution in frequency (velocity); Column 4-7: Observing band, on source time, total observing time and achieved sensitivity per binned channel. The lines without on source time are observed in the same frequency setup as the upper ones with on source time listed in the table.

**Table 2.** Spectral line Observations

Line	$z_{\text{line}}$	FWHM	$S\delta v$	Beam Size	Source Size	Luminosity	Facilities	Ref.
		(km s <sup>-1</sup> )	(Jy km s <sup>-1</sup> )	(arcsec)	(arcsec)	(10 <sup>9</sup> L <sub>⊙</sub> )		
(1)	(2)	(3)	(4)	(5)	(6)	(7)	(8)	(9)
CO (2 – 1)	6.0029 ± 0.0005	484 ± 48	0.18 ± 0.02	0.61 × 0.59	(0.60 ± 0.18) × (0.40 ± 0.21)	0.021 ± 0.002	VLA	S19
CO (5 – 4)	6.0030 ± 0.0004	409 ± 44	0.89 ± 0.09	1.67 × 1.37	-	0.254 ± 0.026	NOEMA	L19
CO (6 – 5)	6.0025 ± 0.0007	456 ± 64	1.52 ± 0.13	5.4 × 3.9	-	0.520 ± 0.045	PdBI	W13
CO (6 – 5)	6.0028 ± 0.0003	361 ± 9	1.12 ± 0.06	0.6 × 0.4	(0.33 ± 0.06) × (0.20 ± 0.04)	0.383 ± 0.021	ALMA	F18
CO (6 – 5)	6.0030 ± 0.0003	422 ± 30	1.05 ± 0.07	1.42 × 1.19	(0.74 ± 0.34) × (0.46 ± 0.28)	0.359 ± 0.024	NOEMA	L19
CO (8 – 7)	6.0028 ± 0.0001	390 ± 15	1.53 ± 0.05	0.79 × 0.75	(0.46 ± 0.09) × (0.21 ± 0.10)	0.699 ± 0.023	ALMA	L19
CO (9 – 8)	6.0031 ± 0.0002	376 ± 18	1.31 ± 0.06	0.77 × 0.63	(0.41 ± 0.10) × (0.32 ± 0.11)	0.673 ± 0.030	ALMA	L19
CO (10 – 9)	-	-	1.04 ± 0.17	-	-	0.594 ± 0.097	-	Rpr
CO (12 – 11)	6.0030 ± 0.0008	451 ± 81	0.78 ± 0.13	2.08 × 1.62	-	0.534 ± 0.089	NOEMA	L19
CO (13 – 12)	6.0028 ± 0.0007	324 ± 75	0.49 ± 0.11	1.91 × 1.53	-	0.363 ± 0.082	NOEMA	L19
H <sub>2</sub> O	6.0028 ± 0.0003	398 ± 28	0.70 ± 0.05	0.72 × 0.68	(0.39 ± 0.14) × (0.25 ± 0.21)	0.343 ± 0.024	ALMA	L19
OH <sup>+</sup>	-	320 ± 313	0.13 ± 0.10	0.77 × 0.63	-	0.067 ± 0.051	ALMA	L19
[CII]158um	6.0031 ± 0.0002	393 ± 21	8.83 ± 0.44	0.72 × 0.51	(0.55 ± 0.05) × (0.40 ± 0.07)	8.310 ± 0.414	ALMA	W13

NOTE—Column 1: Line ID; Column 2 - 4: Redshift, line width in FWHM and line flux. Note that the line flux is calculated through a single Gaussian fit to the line profile; Column 5: Beam size in FWHM; Column 6: Source size deconvolved from the beam in FWHM; Column 7: Line luminosity, and calibration uncertainties are not included in the error bars; Column 8: Facilities; Column 9: References: This paper (L19); Shao et al. (2019) (S18); Wang et al. (2013) (W13); Feruglio et al. (2018) (F18), Riechers et al. in prep (Rpr)

## 7. ACKNOWLEDGEMENT

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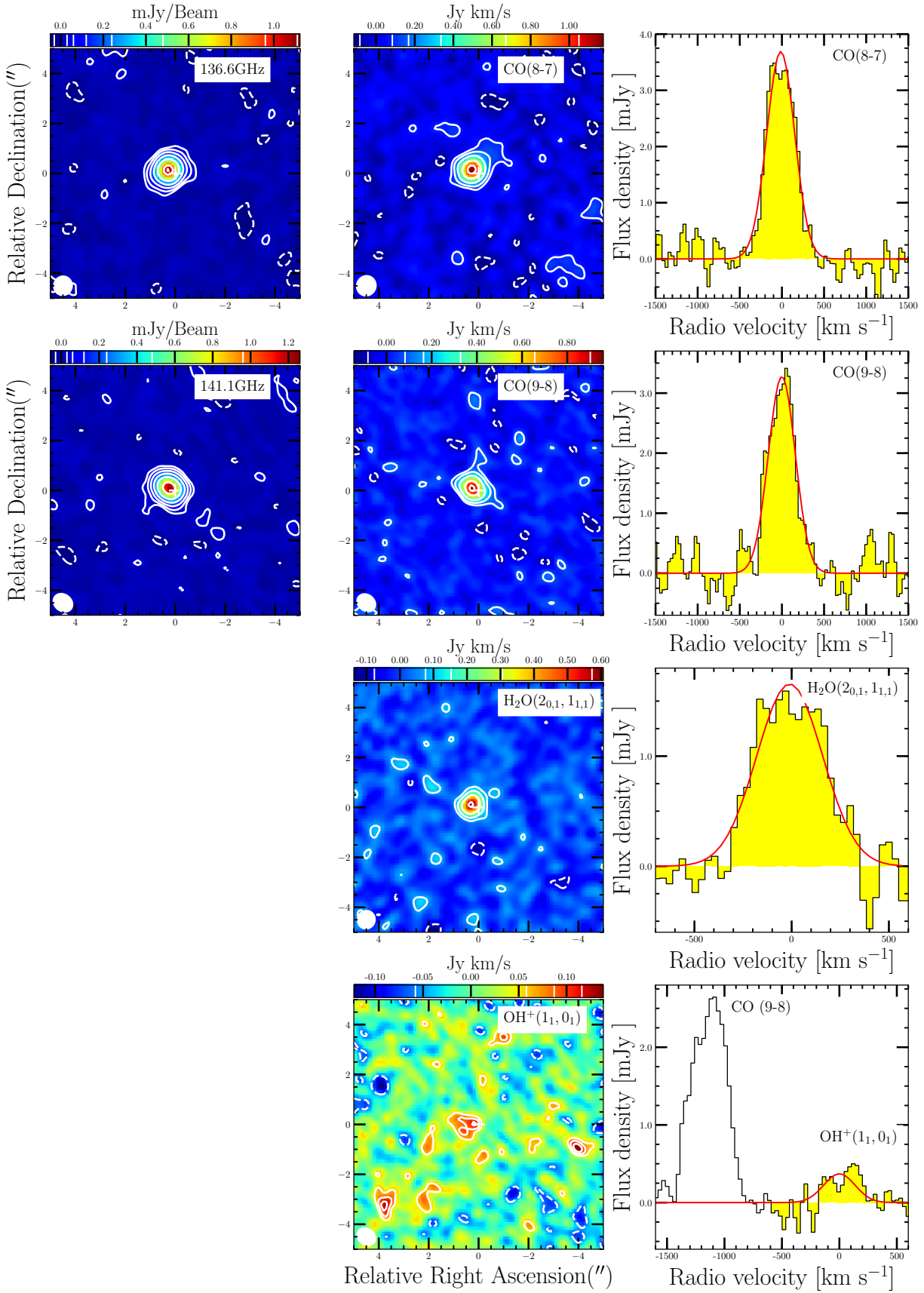


Figure 1. (Caption continued on the next page.)

**Figure 1.** Continuum, line intensity maps, and spectrum (**from left to right**) of CO (8 – 7), (9 – 8), H<sub>2</sub>O(2<sub>0,2</sub> – 1<sub>1,1</sub>) and OH<sup>+</sup>(1<sub>1</sub> – 0<sub>1</sub>) (**from top to bottom**) observed by ALMA. The white cross represents the Gaia position of the quasar (Shao et al. 2019). The size of the white cross demonstrate the astrometric uncertainty of the quasar position. The filled white ellipse on the lower left shows the FWHM of the beam. **First column:** Continuum maps. The white contours denote [-2, 2, 4, 8, 16, 32, 64, 74]×σ (1σ = 15 μJy beam<sup>-1</sup>) at 136.6 GHz and [-2, 2, 4, 8, 16, 32, 64]×σ (1σ = 15 μJy beam<sup>-1</sup>) at 141.1 GHz. **Second column:** Spectra line intensity maps. The white contours denote [-2, 2, 4, 8, 16, 25]×σ (1σ = 0.042 mJy beam<sup>-1</sup> · km s<sup>-1</sup>), [-2, 2, 4, 8, 16, 22]×σ (1σ = 0.041 mJy beam<sup>-1</sup> · km s<sup>-1</sup>), [-2, 2, 4, 8, 15]×σ (1σ = 0.038 mJy beam<sup>-1</sup> · km s<sup>-1</sup>) and [-2, 2, 3, 4]×σ (1σ = 0.029 mJy beam<sup>-1</sup> · km s<sup>-1</sup>) for CO (8 – 7), (9 – 8), H<sub>2</sub>O(2<sub>0,2</sub> – 1<sub>1,1</sub>) and OH<sup>+</sup>(1<sub>1</sub> – 0<sub>1</sub>) respectively. **Third column:** Yellow histogram represents the spectra extracted from the 2 σ contour on the intensity map for spatially resolved CO (8 – 7), (9 – 8), H<sub>2</sub>O(2<sub>0,2</sub> – 1<sub>1,1</sub>) lines, and from the peak pixel for spatially unresolved OH<sup>+</sup>(1<sub>1</sub> – 0<sub>1</sub>) emission. The red solid line is a single Gaussian profile fit to the spectral line. The Gaussian fit to the OH<sup>+</sup>(1<sub>1</sub> – 0<sub>1</sub>) spectral line should be taken with caution since there are possibly both emission and absorption features, and the current sensitivity is not enough to confirm these features. The spatial offsets between the continuum and spectra line emissions are within the uncertainty of the quasar position.

**Table 3.** Continuum Properties

Frequency	Sν	Rms	Beam Size	Source Size
(GHz)	(mJy)	(uJy beam <sup>-1</sup> )	(arcsec)	(arcsec)
(1)	(2)	(3)	(4)	(5)
80.6	0.22 ± 0.04	16	1.68 × 1.37	(1.59 ± 0.52) × (0.21 ± 0.45)
96.0	0.29 ± 0.03	15	1.42 × 1.19	(0.83 ± 0.25) × (0.31 ± 0.39)
136.6	1.28 ± 0.03	15	0.75 × 0.72	(0.34 ± 0.04) × (0.22 ± 0.06)
141.1	1.42 ± 0.03	15	0.80 × 0.65	(0.27 ± 0.03) × (0.22 ± 0.06)
200.9	3.88 ± 0.04	45	2.06 × 1.62	-
215.9	4.46 ± 0.05	45	1.92 × 1.54	-

NOTE—Column 1: Continuum frequency in observed frame; Column 2-3: Continuum flux density and rms; Column 4-5: Beam size and source size deconvolved from beam in FWHM.

**Table 4.** MOLPOP-CEP Grid Parameter Ranges

Input Parameters	Range	Grid Step	Grid Number	Unit
(1)	(2)	(3)	(4)	(5)
Kinetic Temperature ( $T_{\text{kin}}$ )	20 - 800	$\Delta T_{\text{kin}} = 13$	61	K
Volume Density ( $n(\text{H}_2)$ )	$10^3 - 10^8$	$\Delta \text{Log}(n_{\text{H}_2}/\text{cm}^{-3}) = 0.25$	21	cm <sup>-3</sup>
Column Density ( $N(\text{CO})$ )	$10^{14} - 10^{21}$	$\Delta \text{Log}(N_{\text{CO}}/\text{cm}^{-2}) = 0.5$	15	cm <sup>-2</sup>

NOTE—Column 1: Input parameters to generate the grid; Column 2: Parameter ranges; Column 3: Steps of parameters in log space; Column 4: The resulting number of grid for a specific parameter; Column 5: Units

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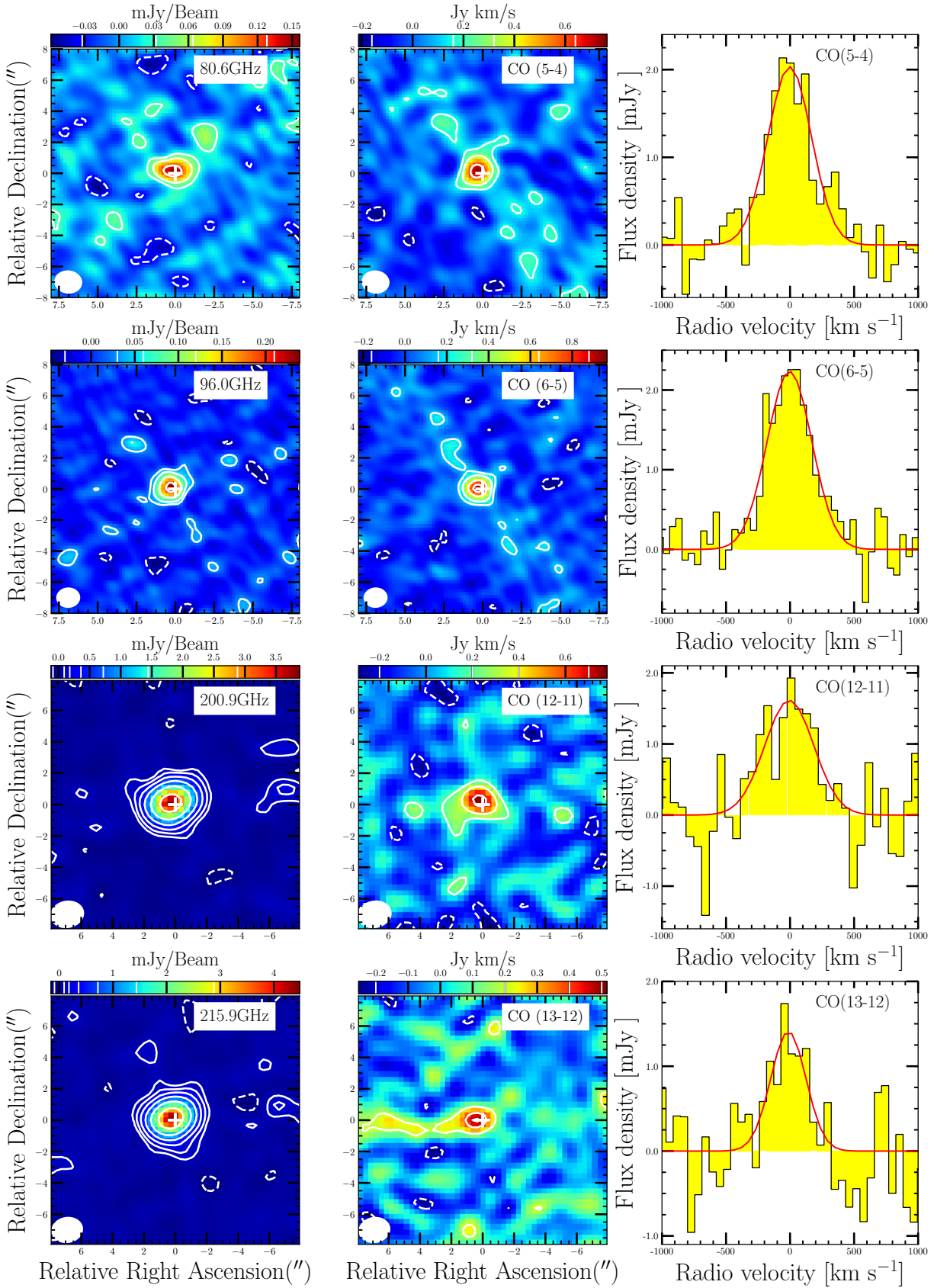
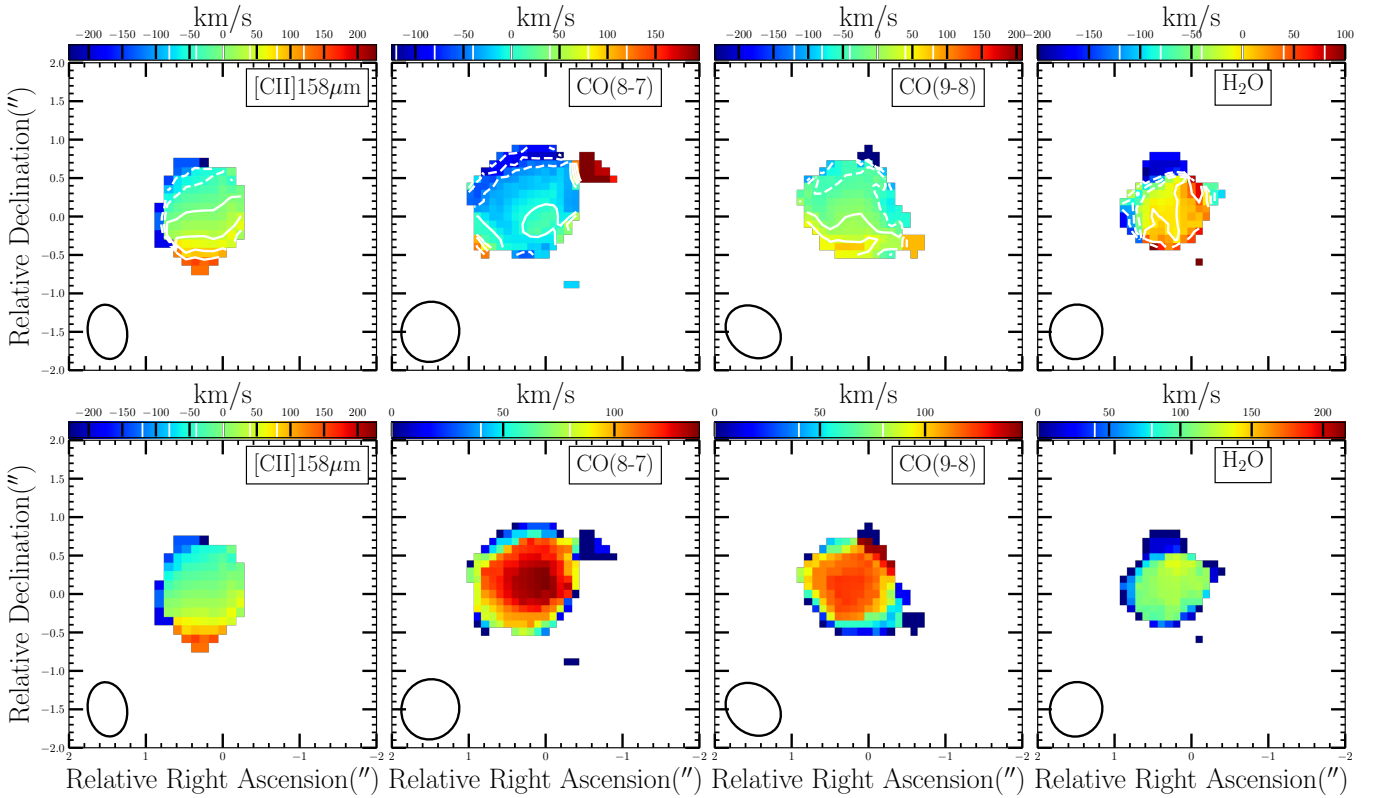
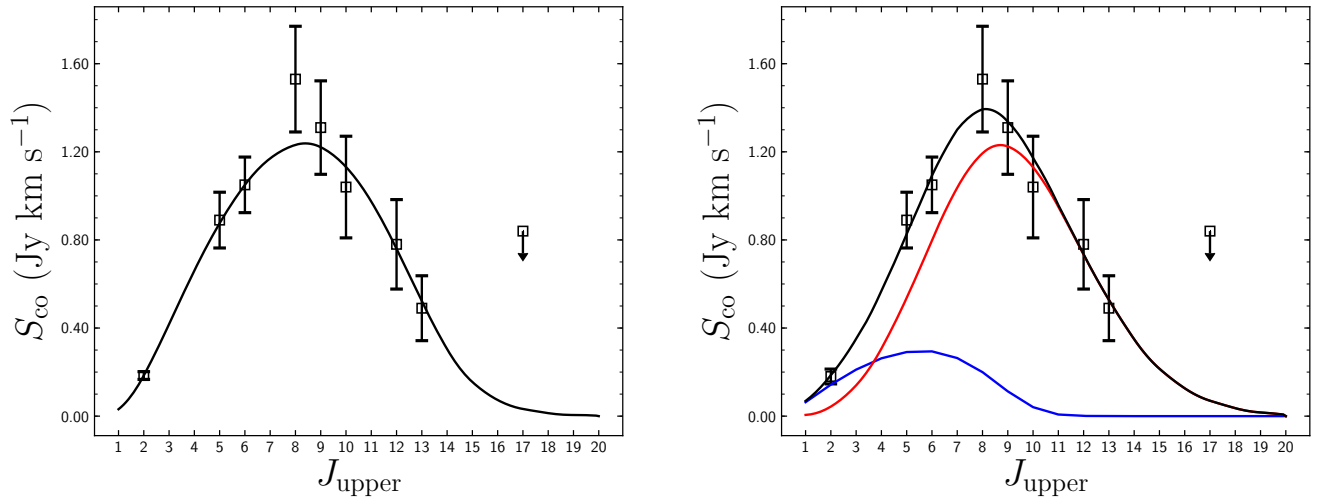


Figure 2. (Caption continued on the next page.)

**Figure 2.** Continuum, line intensity maps, and spectrum (**from left to right**) of CO (5 – 4), (6 – 5), (12 – 11) and (13 – 12) (**from top to bottom**) observed by NOEMA. The white cross on continuum and line intensity map represents the Gaia position of the quasar (Shao et al. 2019). The size of the white cross demonstrates the quasar location astrometric uncertainty. The filled white ellipse on the lower left shows the FWHM of the beam. For the continuum maps (**First column**), contours denote  $[-2, 2, 4, 8] \times \sigma$  ( $1\sigma = 16 \mu\text{Jy beam}^{-1}$ ) at 80.6 GHz,  $[-2, 2, 4, 8, 14] \times \sigma$  ( $1\sigma = 15 \mu\text{Jy beam}^{-1}$ ) at 96.0 GHz,  $[-2, 2, 4, 8, 16, 32, 64] \times \sigma$  ( $1\sigma = 45 \mu\text{Jy beam}^{-1}$ ) at 200.9 GHz and  $[-2, 2, 4, 8, 16, 32, 64] \times \sigma$  ( $1\sigma = 45 \mu\text{Jy beam}^{-1}$ ) at 215.9 GHz. For the spectra line intensity maps (**Second column**), contours denote  $[-2, 2, 4, 8, 10] \times \sigma$  ( $1\sigma = 0.08 \text{ mJy beam}^{-1} \cdot \text{km s}^{-1}$ ),  $[-2, 2, 4, 8, 11] \times \sigma$  ( $1\sigma = 0.08 \text{ mJy beam}^{-1} \cdot \text{km s}^{-1}$ ),  $[-2, 2, 4, 7] \times \sigma$  ( $1\sigma = 0.10 \text{ mJy beam}^{-1} \cdot \text{km s}^{-1}$ ) and  $[-2, 2, 4, 5] \times \sigma$  ( $1\sigma = 0.10 \text{ mJy beam}^{-1} \cdot \text{km s}^{-1}$ ) for CO (5 – 4), (6 – 5), (12 – 11) and (13 – 12) respectively. **Third column:** Yellow histogram represents spectrum extracted from the peak pixel (all spectra lines are spatially unresolved), and the red solid line is a single Gaussian profile fit to the spectral line. The peak positions of the continuum and spectra line emissions are within uncertainty of the quasar position.



**Figure 3.** Velocity (**first row**) and velocity dispersion (**second row**) of [C II]  $158\mu\text{m}$ , CO (8 – 7), (9 – 8) and  $\text{H}_2\text{O}(2_{0,2} - 1_{1,1})$  (Left to right). The black ellipse on the left shows the FWHM of the beam. We generate the velocity and velocity dispersion maps with the pixels of  $\geq 3.0\sigma$  values in the line emitting channels, and the zero velocity corresponds to the [C II]  $158\mu\text{m}$  redshift of 6.0031 (Wang et al. 2013). White contours on the velocity maps are  $[-4, -2, 0, 2, 4, 6] \times 20 \text{ km s}^{-1}$  for [C II]  $158\mu\text{m}$ ,  $[-6, -4, -2, 0, 2, 4, 6] \times 20 \text{ km s}^{-1}$  for CO (8 – 7),  $[-6, -4, -2, 0, 2, 4] \times 20 \text{ km s}^{-1}$  for CO (9 – 8), and  $[-6, -4, -2, 0, 2, 4] \times 20 \text{ km s}^{-1}$  for  $\text{H}_2\text{O}(2_{0,2} - 1_{1,1})$ . We find in the velocity maps that CO (8 – 7), (9 – 8) and  $\text{H}_2\text{O}(2_{0,2} - 1_{1,1})$  generally follow the velocity gradient observed from [C II]  $158\mu\text{m}$  (Wang et al. 2013) from northeast to southwest.



**Figure 4.** CO SLED fitted with one (**left**) or two component (**right**) models. Black squares are the CO fluxes of J2310+1855 with the calibration uncertainties included. The CO (5 – 4), (6 – 5), (8 – 7), (9 – 8), (12 – 11) and (13 – 12) data are from this work. The CO (2 – 1) data is taken from [Shao et al. \(2019\)](#), the CO (10 – 9) data will be presented in [Riechers et al. \(in prep\)](#), and the upper limit of the CO (17 – 16) line is from [Carniani et al. \(2019\)](#). Details are presented in Table 2. **Left:** Black solid line represents the best one-component fitting result with the minimum  $\chi^2$  ( $T_{\text{kin}} = 228$  K,  $\log(n(\text{H}_2)/\text{cm}^{-3}) = 4.75$  and  $\log(N(\text{CO})/\text{cm}^{-2}) = 17.5$ ). **Right:** Least squares fitting result with two-component model. Blue solid line represents the J1148+5251 model with  $T_{\text{kin}} = 50$  K,  $\log(n(\text{H}_2)/\text{cm}^{-3}) = 4.20$  and  $\log(N(\text{CO})/\text{cm}^{-2}) = 18.0$  ([Riechers et al. 2009](#)). Red solid line is the “warm” component with  $T_{\text{kin}} = 306$  K,  $\log(n(\text{H}_2)/\text{cm}^{-3}) = 5.25$  and  $\log(N(\text{CO})/\text{cm}^{-2}) = 15.5$ .

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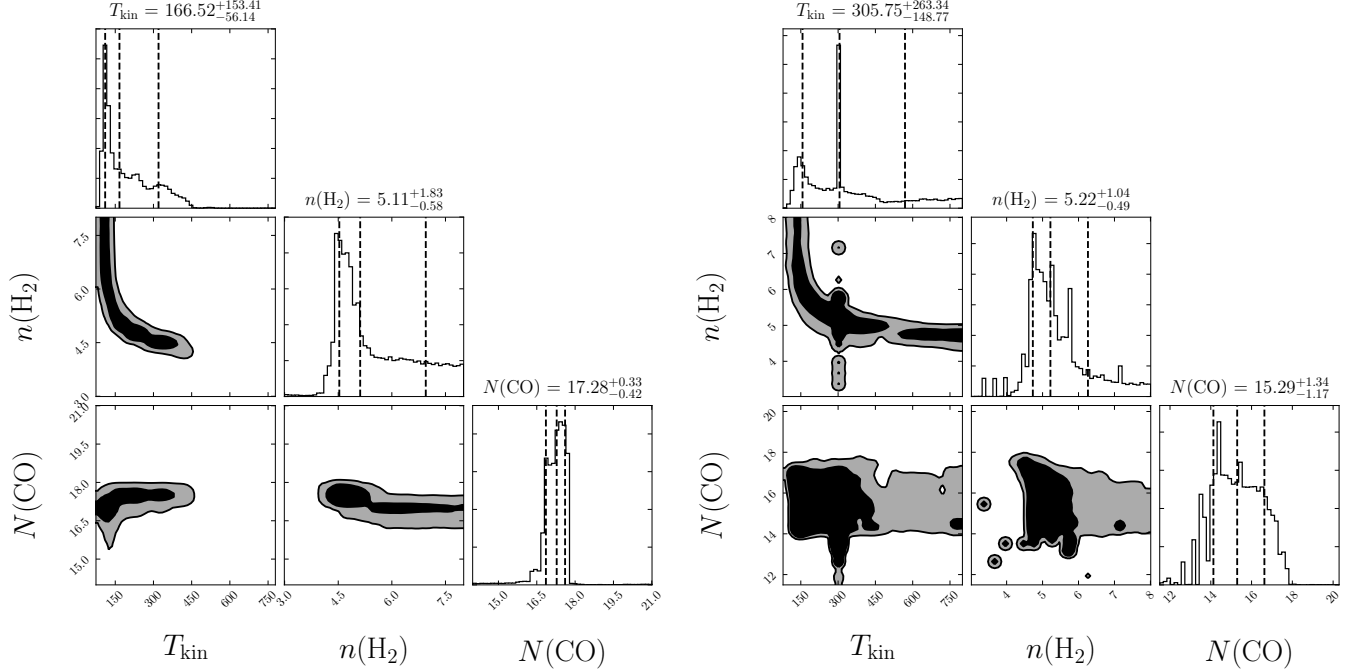
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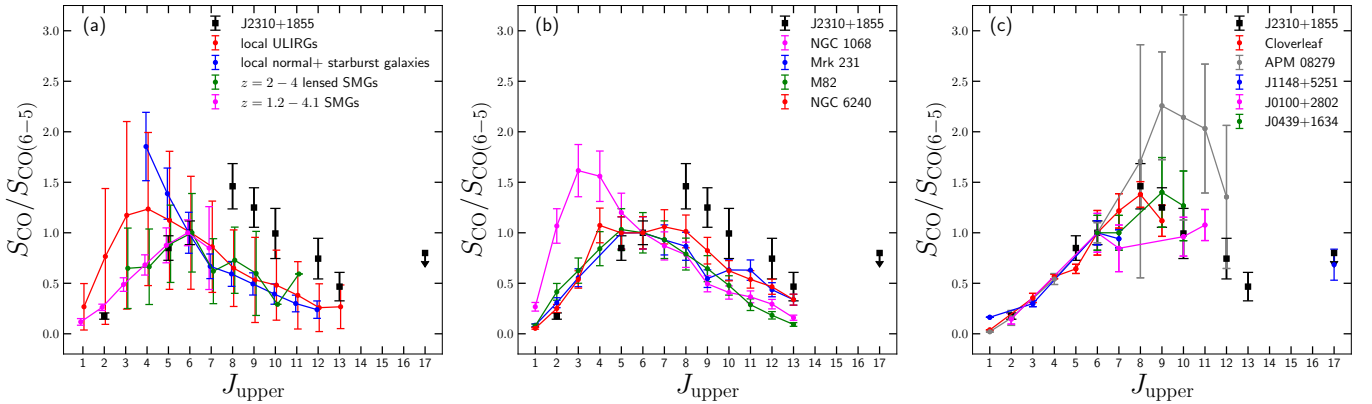
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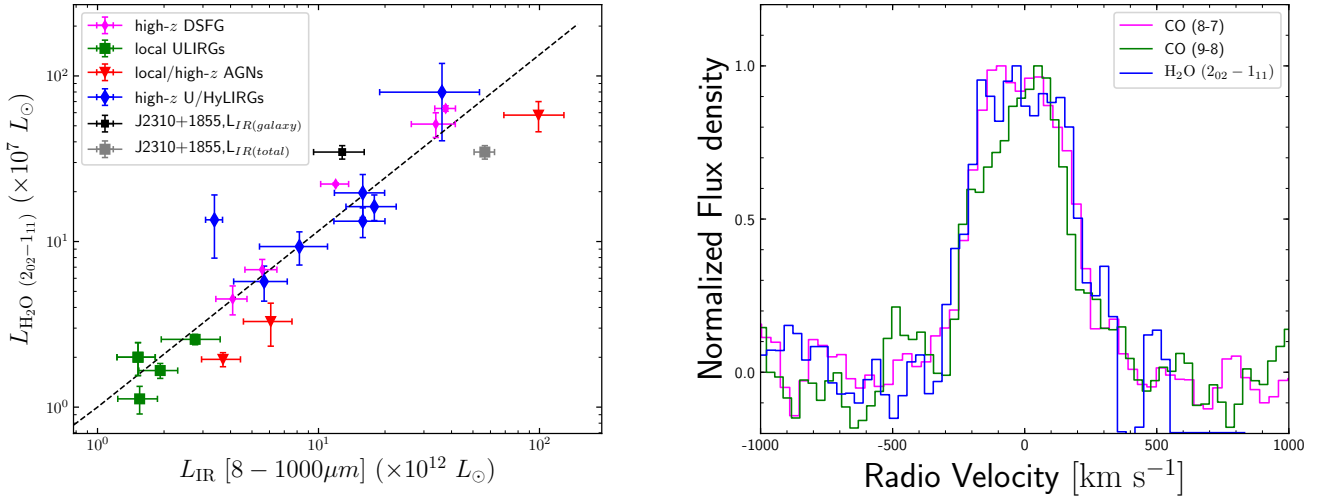
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**Figure 5.** Posterior probability distributions of the three parameters  $T_{\text{kin}}$  (K),  $\log(n(\text{H}_2)/\text{cm}^{-3})$  and  $\log(N(\text{CO})/\text{cm}^{-2})$ . The plotted contours show 95 % and 68 % confidence intervals. **Left:** Posterior probability distribution of the parameters for the one component model. The resulting MCMC result is  $T_{\text{kin}} \approx 167_{-56}^{+153}$  K,  $\log(n(\text{H}_2)/\text{cm}^{-3}) \approx 5.11_{-0.58}^{+1.83}$  and  $\log(N(\text{CO})/\text{cm}^{-2}) \approx 17.28_{-0.42}^{+0.33}$ . We note that the median and uncertainties here are calculated based on the 16th, 50th, and 84th percentiles of the samples in the marginalized distributions. **Right:** Posterior probability distribution of the “warm” component in the two-component model fit to the data. The fitting result suggests the “warm” component with  $T_{\text{kin}} \approx 306_{-149}^{+263}$  K,  $\log(n(\text{H}_2)/\text{cm}^{-3}) \approx 5.22_{-0.49}^{+1.04}$  and  $\log(N(\text{CO})/\text{cm}^{-2}) \approx 15.29_{-1.17}^{+1.34}$ .



**Figure 6.** CO SLED normalized to CO (6–5) in normalized unit of  $\text{Jy km s}^{-1}$ . **Left column:** J2310+1855 (black squares) in comparison with the mean of four galaxy samples: the local (U)LIRGs (Rosenberg et al. 2015) (red); local normal + starburst galaxies (Liu et al. 2015) (blue);  $z \sim 1.2 - 4.1$  SMGs (Bothwell et al. 2013) (magenta); strongly lensed SMGs at  $z \sim 2 - 4$  (Yang et al. 2017) (green). **Middle column:** J2310+1855 (black squares) in comparison with local starburst systems and AGNs. M82 (Panuzzo et al. 2010; Weiß et al. 2005) (green) is a representative example of the local starburst galaxy. The local representative AGNs are NGC 1068 (Spinoglio et al. 2012) (magenta), Mrk231 (van der Werf et al. 2010) (blue) and NGC 6240 (Rosenberg et al. 2015) (red). **Right column:** J2310+1855 (black squares) in comparison with high redshift quasars. The plotted quasars are APM 08279+5255 (Bradford et al. 2011; Weiß et al. 2007; Riechers et al. 2009) (grey), Cloverleaf (Bradford et al. 2009; Uzgil et al. 2016) (red), J1148+5251 (Bertoldi et al. 2003; Walter et al. 2003; Beelen et al. 2006; Riechers et al. 2009; Gallerani et al. 2014) (blue), J0439+1634 (Yang et al. 2019) (green) and J0100+2802 (Wang et al. 2019) (magenta).



**Figure 7. Left:**  $L_{\text{H}_2\text{O}(20,2-11,1)}$  vs  $L_{\text{IR}}$  (from Fig.3 in Yang et al. 2016). The green squares are the local ULIRGs from Yang et al. (2013), the blue diamonds are the high redshift U/HyLIRGs from Yang et al. (2016), Omont et al. (2013), and van der Werf et al. (2011), the magenta diamonds are the high redshift (dusty) star forming galaxies from Jarugula et al. (2019) and Apostolovski et al. (2019), and the red down-triangles represent local and high redshift AGNs, namely Mrk 231 (González-Alfonso et al. 2010), SDP81 (Yang et al. 2016) and APM 08279+5255 (Bradford et al. 2011) from left to right. Note that all the luminosities plotted are intrinsic luminosities that have been corrected for lensing. The grey and black squares mark two cases of J2310+1855: the former (grey square) is the water line to total infrared luminosity ratio with  $L_{\text{IR}(\text{total})} = (5.7 \pm 0.6) \times 10^{13} L_\odot$  (with contributions from both quasar and host galaxy), and the latter (black square) shows the water line to galaxy infrared luminosity ratio with  $L_{\text{IR}(\text{galaxy})} = (1.4 \pm 0.3) \times 10^{13} L_\odot$  (which is purely from the host galaxy). The black dashed line represents the best fit to the local & high  $z$  U/HyLIRGs (green squares and blue diamonds) with  $L_{\text{H}_2\text{O}(20,2-11,1)} \sim L_{\text{IR}}^{1.06}$ , see (Yang et al. 2016). Note that the definition of infrared luminosity is 8 – 1000  $\mu\text{m}$ . **Right:** Spectrum of CO (8 – 7) (magenta), (9 – 8) (green) and H $_2$ O(20,2 – 11,1) (blue) normalized to the peak flux densities.

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