

 Open access • Journal Article • DOI:10.1088/0004-637X/723/2/1139

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Andrew I. Harris, Andrew J. Baker, S. G. Zonak, Chelsea E. Sharon ...+4 more authors

Institutions: University of Maryland, College Park, Rutgers University, Max Planck Society, National Radio Astronomy Observatory

Published on: 10 Nov 2010 - The Astrophysical Journal (IOP Publishing)

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CO $J = 1-0$ SPECTROSCOPY OF FOUR SUBMILLIMETER GALAXIES WITH THE ZPECTROMETER ON THE GREEN BANK TELESCOPE

A. I. HARRIS¹, A. J. BAKER², S. G. ZONAK¹, C. E. SHARON², R. GENZEL^{3,4}, K. RAUCH¹, G. WATTS⁵, AND R. CREAGER⁵

¹ Department of Astronomy, University of Maryland, College Park, MD 20742, USA; harris@astro.umd.edu, szonak@astro.umd.edu, rauch@astro.umd.edu

² Department of Physics and Astronomy, Rutgers, The State University of New Jersey, Piscataway, NJ 08854-8019, USA; ajbaker@physics.rutgers.edu, csharon@physics.rutgers.edu

³ Max-Planck-Institut für Extraterrestrische Physik, Giessenbachstrasse 1, D-85741 Garching, Germany; genzel@mpe.mpg.de

⁴ Department of Physics, Le Conte Hall, University of California, Berkeley, CA 94720, USA

⁵ National Radio Astronomy Observatory, P.O. Box 2, Green Bank, WV 24944, USA; gwatts@nrao.edu, rcreager@nrao.edu

Received 2010 June 16; accepted 2010 September 6; published 2010 October 19

ABSTRACT

We report detections of three $z \sim 2.5$ submillimeter-selected galaxies (SMGs; SMM J14011+0252, SMM J14009+0252, SMM J04431+0210) in the lowest rotational transition of the carbon monoxide molecule (CO $J = 1-0$) and one nondetection (SMM J04433+0210). For the three galaxies we detected, we find a line-integrated brightness temperature ratio of the $J = 3-2$ and $1-0$ lines of 0.68 ± 0.08 ; the $1-0$ line is stronger than predicted by the frequent assumption of equal brightnesses in the two lines and by most single-component models. The observed ratio suggests that mass estimates for SMGs based on $J = 3-2$ observations and $J = 1-0$ column density or mass conversion factors are low by a factor of 1.5. Comparison of the $1-0$ line intensities with intensities of higher- J transitions indicates that single-component models for the interstellar media in SMGs are incomplete. The small dispersion in the ratio, along with published detections of CO lines with $J_{\text{upper}} > 3$ in most of the sources, indicates that the emission is from multi-component interstellar media with physical structures common to many classes of galaxies. This result tends to rule out the lowest scaling factors between CO luminosity and molecular gas mass, and further increases molecular mass estimates calibrated against observations of galaxies in the local universe. We also describe and demonstrate a statistically sound method for finding weak lines in broadband spectra that will find application in searches for molecular lines from sources at unknown redshifts.

Key words: galaxies: high-redshift – galaxies: individual (SMM J04431+0210, SMM J04433+0210, SMM J14011+0252, SMM J14009+0252) – galaxies: ISM – methods: statistical – techniques: spectroscopic

1. INTRODUCTION

Observations and models of the extragalactic far-infrared/submillimeter background (e.g., Puget et al. 1996; Fixsen et al. 1998; Lagache et al. 2003) indicate that a large fraction of cosmic star formation has taken place behind a veil of dust. At high redshift, this conclusion is consistently affirmed by comparisons of obscured and unobscured star formation in optically selected galaxy populations (e.g., Reddy et al. 2008). A more striking pattern emerges when one considers *all* galaxy populations, however: the systems forming stars at the highest rates (i.e., having the highest bolometric luminosities) are also the dustiest (Adelberger & Steidel 2000). This trend reaches an extreme in the case of submillimeter galaxies (SMGs), first identified over a decade ago as bright (>5 mJy) sources in $850 \mu\text{m}$ surveys with the Submillimeter Common-user Bolometer Array (SCUBA) on the James Clerk Maxwell Telescope (e.g., Smail et al. 1997; Barger et al. 1998; Hughes et al. 1998). SMGs have faint X-ray counterparts (Alexander et al. 2005) and show the disturbed morphologies characteristic of major mergers (Conselice et al. 2003, cf. Davé et al. 2010), suggesting they are important sites of mass assembly as well as star formation. However, their high obscuration has also proved challenging for detailed study, including determining their precise redshifts and masses, and understanding their interstellar media and star formation processes. While photometric techniques shed some light on SMGs' redshift distribution (e.g., Aretxaga et al. 2003), obtaining more than a handful of spectroscopic redshifts for SMGs and their warmer analogs has required a painstaking effort of radio continuum mapping followed by optical spec-

troscopy (Chapman et al. 2003, 2004, 2005), whose results have been securely confirmed by the detection of CO emission lines at millimeter wavelengths (Neri et al. 2003; Greve et al. 2005; Tacconi et al. 2006; Chapman et al. 2008; Bothwell et al. 2010).

Redshift determination is the first step toward addressing the crucial question of SMGs' masses. Translation of SMGs' angular clustering strength (Blain et al. 2004; Weiß et al. 2009b) to a linear correlation length and dark matter halo mass depends sensitively on their exact redshift distribution, although a large characteristic halo mass can be independently estimated from cosmological simulations assuming a proportionality between dark matter accretion and star formation rates (Genel et al. 2008). The total dynamical masses of the galaxies themselves are also large, as first suggested by measurements of large CO linewidths (e.g., Frayer et al. 1998, 1999) and confirmed by spatially resolved CO mapping (e.g., Downes & Solomon 2003; Genzel et al. 2003; Tacconi et al. 2006, 2008; Bothwell et al. 2010). However, given the challenges of obtaining such mapping and the complications of high extinction for stellar mass determinations (e.g., Hainline et al. 2010), estimating SMGs' molecular gas masses from their CO line luminosities remains a useful way to place lower limits on their total masses. Accurate molecular gas masses are also required to determine SMGs' gas mass fractions and star formation efficiencies, important inputs for understanding their evolutionary status and the likely properties of their descendants (Baugh et al. 2005; Swinbank et al. 2009).

In this paper, we report observations of four SMGs, drawn from the SCUBA Lens Survey (SLS) sample of Smail et al.

(2002), with the ultrawide-bandwidth Zpectrometer cross-correlation spectrometer on the 100 m diameter Robert C. Byrd Green Bank Telescope (GBT). For the three of our targets that are brightest at 850 μm , the Zpectrometer has successfully detected the lowest ($J = 1-0$) rotational transition of carbon monoxide (CO), and we undertake a joint analysis with published CO $J = 3-2$ detections for this trio of massive SMGs at $z \sim 2.5$.

Studies of our own and nearby galaxies have established the CO $J = 1-0$ line ($\nu_{\text{rest}} = 115.27$ GHz) as a proxy for tracing the molecular hydrogen (H_2) that forms giant molecular clouds. CO is the most abundant molecule after H_2 and, unlike H_2 , has a permanent dipole moment that allows it to radiate efficiently. The magnitude of the molecule's dipole moment and close spacing between the lowest rungs of its rotational ladder allow it to be collisionally excited to trace gas particle densities above a few hundred per cubic centimeter and temperatures above 5 K. The strong C–O bond helps keep the molecule stable against dissociation by ultraviolet light and shocks, so CO probes active as well as quiescent regions. Transitions between rotational states with increasing rotational quantum number J trace increasingly warm and dense gas. Rest-frame submillimeter lines trace particle densities of $\sim 10^4\text{--}10^5$ cm^{-3} and kinetic temperatures of several tens to a few hundred kelvins.

For all its advantages as a molecular gas tracer, observations of the $J = 1-0$ transition at high redshift have been hampered by its relatively low observed frequency. Observations of the line are rapidly becoming easier as technology improves, as the run of publication dates for detections of galaxies at $z > 1$ shows (Papadopoulos et al. 2001; Greve et al. 2003; Klamer et al. 2005; Hainline et al. 2006; Riechers et al. 2006; Swinbank et al. 2010; Carilli et al. 2010; Ivison et al. 2010a, 2010b; Aravena et al. 2010; Negrello et al. 2010; Frayer et al. 2010). Peak flux density from optically thick and thermalized emission scales roughly as frequency squared, so the 1–0 lines from distant galaxies are expected to be an order of magnitude weaker than the 3–2 and other mid- J lines from the same sources. The 100 m diameter GBT combines an enormous collecting area and a low centimeter-wave system temperature to approach the necessary sensitivity level. Stability is a key consideration for long integrations, and motivated our construction of the Zpectrometer, a cross-correlation spectrometer optimized for line searches that instantaneously covers the GBT Ka -band receiver's 25.6–36 GHz band. In this band, the CO $J = 1-0$ line redshifts over a $2.2 \leq z \leq 3.5$ range that includes the peak of the Chapman et al. (2005) SMG redshift distribution. The Zpectrometer and correlation receiver architecture have improved stability to the point that detection of 1–0 emission is relatively straightforward for sources with extreme ($\mathcal{M} \gtrsim 10$) magnifications due to gravitational lensing (Swinbank et al. 2010; Negrello et al. 2010; Frayer et al. 2010). In this paper, we discuss observations of weaker CO 1–0 lines from galaxies that have considerably less magnification than the brightest sources.

The prime goal of our observations was to measure the ratios of 1–0 to higher- J line fluxes to explore the physical conditions in our targets' molecular gas and to test standard assumptions in the use of empirical conversion factors to relate their CO luminosities to their molecular gas masses. CO $J = 1-0$ spectra of these galaxies are especially important because they constrain the state of their molecular interstellar media and may reveal the presence of massive reservoirs of extended cool gas that do not appear in lines from more excited states. In addition to tracing

cool gas, the 1–0 line is essential for interpreting mid- J lines to constrain the properties of warmer gas. In the local universe, multi-line observations of nearby starburst and active galactic nuclei typically show low- and high-excitation gas components (e.g., Wild et al. 1992; Guesten et al. 1993; Mao et al. 2000; Ward et al. 2003; Greve et al. 2009), with the two components distinct in low- and high- J lines but contributing jointly to mid- J lines. Fluxes in the 1–0 and 2–1 lines are essential for characterizing the cool component well enough to determine the fraction of the mid- J emission that comes from each component.

A secondary outcome of our observations was to test the use of the Zpectrometer's large fractional bandwidth ($\Delta f/f_{\text{mean}} = 34\%$) for blind redshift searches toward targets identified in continuum surveys. The Zpectrometer's instantaneous redshift coverage is 5–10 times larger than those provided by current millimeter-wave interferometer bandwidths, offering the promise of quick CO redshift determinations for SMGs without waiting for radio continuum mapping or optical spectroscopy. To that end, we developed a statistical test for line detection appropriate for long observations across wide bandwidths. The ability to identify sources directly from continuum positions known to within the 22'' size of the GBT's Ka -band beam eliminates some selection effects that bias detection toward excited molecular gas.

This paper has three further sections and an appendix. Section 2 describes our observational technique and instrument. Section 3 covers our basic results for each source, including an overview of a detection method suitable for wideband spectroscopy. Section 4 contains discussion of the physical conditions in the galaxies we detected, the implications, and a brief summary. The Appendix describes the details of the detection statistic whose use we demonstrate here.

2. OBSERVATIONS

The combination of the Zpectrometer cross-correlation spectrometer and dual-channel Ka -band correlation receiver is specifically intended for wideband observations of weak lines. The system's use of correlation makes it the single-dish equivalent of a two-element spatial interferometer (Blum 1959; Harris 2005), with a similar promise for high stability. The spectrometer has moderate velocity resolution that is well matched to extragalactic observations: its spectral response to a monochromatic line is a $\text{sinc}(x)$ function with 20 MHz FWHM, corresponding to about 190 km s^{-1} at band center. A correlation spectrometer is immune to some systematic effects in line detection experiments, as the narrow spectral feature corresponding to a line is not produced by a single detector, but is created by coherent structure across hundreds of independent lags.

Physically, the Zpectrometer analog lag cross-correlator is installed next to the Ka -band receiver on the National Radio Astronomy Observatory's 100 m diameter GBT (Harris et al. 2007). Even in a digital age, analog multiplication still retains advantages of low power dissipation and low radiated emissions for broadband spectroscopy. Transistor analog multipliers separated by transmission line delays cascade to form the Zpectrometer's lag correlators. Sets of 256 lags are packaged in four identical independent cross-correlator units, each with 3.5 GHz bandwidth. A four-channel downconverter splits the receiver's IF band to stack the correlators in frequency space. Receiver performance at high frequency limits the bandwidth, so the spectra in this paper cover 10.5 GHz, the three lowest-frequency correlator sub-bands. Harris (2005) covers the details

of how the combination of a correlation receiver front end and analog lag cross-correlator back end differences the power between the receiver’s two input feed horns. This electronic differencing greatly reduces the effects of amplifier $1/f$ gain noise, the dominant source of instability in good total power radiometers. Layers of optical switching (chopping, wobbling, nodding, beamswitching, double-beamswitching, etc.; the terminology is mixed) and electronic phase switching remove other nonideal signals to a very high degree, leaving spectra that are very clean compared with a conventional total power system.

While the correlation architecture greatly improved stability, switching the beam position on the sky by moving the telescope subreflector (chopping) at a 10 s period was still necessary for usable stability. A chop throw of 78 arcsec, equal to the angular separation of the correlation receiver’s two feed horns, alternately placed the source on one of the two horns, optically switching the source between the receiver’s “plus” and “minus” sense beams. Differencing the spectra from the two subreflector positions (tilts) reduced electronic imbalances, but the slight difference in telescope illumination in the two subreflector positions introduced spectral structure from optical imbalance with a peak–peak amplitude of approximately 60 mJy. Changing the antenna position to view a reference position on the nearby sky and then differencing these “source” and “reference” subreflector-switched spectra removed the optical imbalance to a high degree. This is the classical double-beamswitching or chop-and-nod pattern common to short-wavelength radio and infrared astronomy; we used an 8 minute cycle time and telescope moves of no more than a few degrees. Rather than spending half of the time observing blank sky, we took advantage of the system’s fixed-tuned operation and wide bandwidth by switching between two sources close in sky positions. This increases observing efficiency by a factor of two at the cost of not preserving individual source continuum levels, and risking that lines from the two sources will fall at the same frequencies and cancel to a greater or lesser extent. We felt the gain in time offset the risk, and we preserved the data from each chop side to recover from this eventuality. Residual imbalance in the receiver caused some fluctuating large-scale structure and an occasionally strong ripple across the spectral baseline on timescales short compared with the optical switching times. While this structure tended to cancel after long integrations, it was still present in the spectrum and added nonideal noise. Although the noise amplitude in spectra decreased as the square root of integration time, excess noise in the receiver was a factor of two to four higher than the radiometer equation predicts.

We made gain corrections across the band and established the intensity scale by dividing the source minus reference spectra by spectra of the standard radio flux calibrators obtained in the same observing sessions. We took absolute fluxes of 0.77 and 1.9 Jy at 32.0 GHz for 3C48 and 3C286 from The Astronomical Almanac. Observations of Mars, compared against a physical model for Mars’ emission (B. Butler 2009, private communication), independently verified the flux scale within a few percent and established the quasars’ spectral indices across the band. We tracked the total power at the Zpectrometer’s four-channel downconverter to monitor the system temperature, but system temperature measurements were complicated by the presence of nonideal phase noise, which does not appear in total power.

Stepping monochromatic signals with 8 MHz spacings across the receiver band calibrated the system phase and established the correlator’s spectral frequency scale (Harris & Zmuidzinas 2001; Harris 2005). Signals from one of the GBT’s microwave

Table 1
Summary of Observations

Name	R.A. (J2000)	Decl. (J2000)	No. Sessions	t_{int}
SMM J04431+0210	04:43:07.10	+02:10:25.1	9	9.8
SMM J04433+0210	04:43:15.00	+02:10:02.0		
SMM J14011+0252	14:01:04.96	+02:52:23.5	3	3.1
SMM J14009+0252	14:00:57.68	+02:52:48.6		

Notes. A horizontal line separates the pairs of sources that were observed together. The total integration time t_{int} is the elapsed observing time for each of the difference spectra (Figures 1 and 4).

synthesizers were injected between one of the feed horns and the receiver’s input hybrid for this purpose. To simplify this phase calibration, the system local oscillators run at fixed frequencies, so the system frequency scale is topocentric. Doppler shift corrections to bring the velocity scale to a local standard of rest (LSR) scale were applied in data reduction. We used version D of the Zpectrometer’s data reduction pipeline, written in GBTIDL (Marganian et al. 2006), to make calibrated spectra and quick-look evaluation during observations. Further data analysis was in R language (R Development Core Team 2006) routines.

The telescope pointing was generally excellent when the wind was low ($\leq 3 \text{ m s}^{-1}$) and for elevations between 75° and 20° . We pointed on a compact source near the astronomical targets once per hour, finding typical corrections of 0.1 arcmin or below, or about a third of the 0.35 arcmin beamwidth (0.84 of the peak amplitude for a Gaussian beam) at 30 GHz.

We took spectra of the pointing source hourly to monitor systematic gain changes and periodically monitored receiver gain with a modulated noise source at its input. Optical gain changes from pointing and focus errors were dominant, and we found that the systematic overall calibration drifted by a maximum of 20% over an hour, less at lower frequencies than high. The drifts produced a bias that could slightly underpredict CO $J = 1-0$ line strengths.

3. RESULTS

We observed the sources in pairs to cancel optical offsets, as described in Section 2, so we summarize the results by pairs of sources. Positions, numbers of observing sessions, and total integration times t_{int} for each pair are listed in Table 1.

Our data analysis for the spectra in this paper is untuned: we used an unweighted average of all the data from all of the sessions for all sources. Time-varying nonideal noise dominated the spectral structure, so weighting by system temperature was not appropriate, and ad hoc weighting or editing based on measured session fluctuations or structure in individual spectra was not justified. No baseline structure has been removed other than narrowband filtering in the Fourier domain to remove an approximately 300 MHz period ripple produced in the receiver. Offsets from zero flux density in the spectra are reproducible but are different for different source pairs: they give the continuum level differences between the sources in the pairs. There is no sign of discontinuity between the three correlator sub-bands, even on strong continuum sources, a sign that the correlator’s response is very linear in power.

3.1. SMM J14011+0252 and SMM J14009+0252

The upper panel of Figure 1 is the full-band difference spectrum between this pair of sources, showing detections for

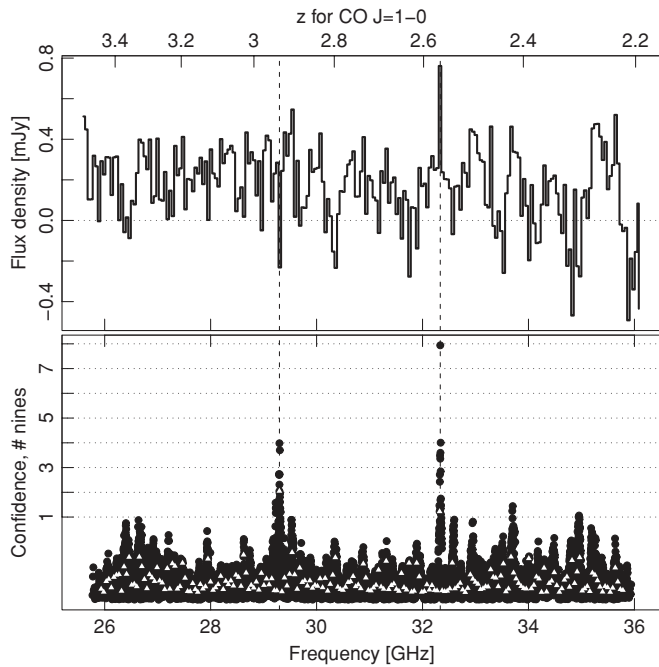


Figure 1. Difference spectrum of SMM J14011+0252 and SMM J14009+0252 (upper panel) and confidence plot (lower panel). The triangles in the confidence plot mark the points corresponding to the binning for the spectrum in the top panel. As is apparent from the position of the triangles in the confidence plot, the binning for the top spectrum is the compromise necessary to show SMM J14011+0252’s narrow line and SMM J14009+0252’s broader line, so this spectrum shows neither line detection to its best advantage. In the confidence plot, the ordinate gives the number of nines (0.9, 0.99, etc.) in the confidence level; see the text.

both: a positive spike corresponds to an emission line from the first source of the pair, SMM J14011+0252 at $z \sim 2.55$, and a negative-going spike corresponds to emission from the second source, SMM J14009+0252 at $z \sim 2.95$. The binning in the top panel of Figure 1 does neither source justice because it is a compromise between that best suited to the detection of J14011+0252’s narrow line and J14009+0252’s broad line.

The lower panel in the figure contains a summary of many possible binnings and shows the detections much more clearly. We identify lines by exploiting the fact that even broad extragalactic lines are narrow on the scale of the Zpectrometer’s bandwidth, searching for a relatively narrow peak across a spectrum whose noise changes with frequency. This is a detection confidence plot, a statistically sound quantitative embodiment of what an experienced observer would do by eye: look to see whether a spectral channel or set of channels is higher than its neighbors, within fluctuations. Estimating noise levels by eye is complicated by the changes in noise across the spectrum’s 25.6–36 GHz band; the fluctuation across all channels is not a good measure of the fluctuations within individual channels. Points in the figure summarize the results from our detection statistic, which is described in the Appendix, over a wide range of binning parameters. Each dot in the confidence plot represents the result from the detection statistic for one combination of bin width and start channel index for the binning. In Figure 1 (and Figure 4), bin widths run from $n = 3$ to 10 and starting bins run from 0 to $n - 1$. The triangles mark dots corresponding to the bin width and starting bin for the spectrum in the top panel, with one triangle at the center of each frequency bin. Columns of dots are frequencies where the detection statistic is high for a range of bin widths and center offsets. Isolated

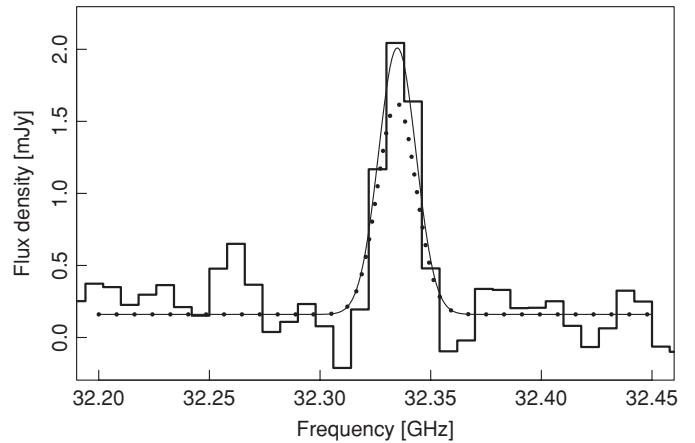


Figure 2. Spectrum of SMM J14011+0252 with Gaussian profile fit (curve) and Gaussian equivalent of the 3–2 spectral fit with flux density divided by nine (dotted; Downes & Solomon 2003).

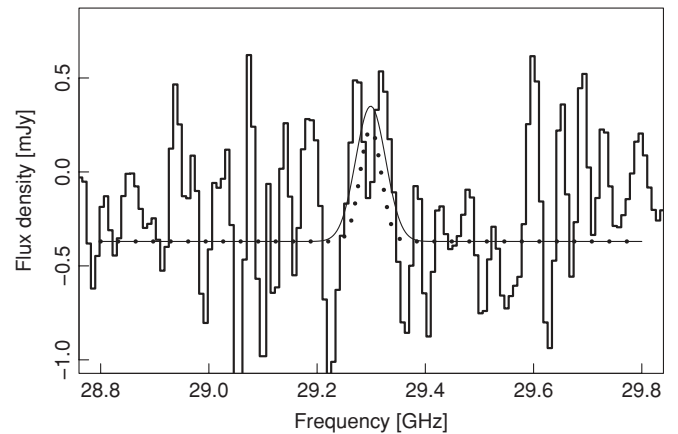


Figure 3. Spectrum of SMM J14009+0252 with Gaussian profile fit (curve) and Gaussian equivalent of the 3–2 spectral fit with flux density divided by nine (dotted; Weiß et al. 2009a).

dots are most likely to be chance fluctuations emphasized by a particular set of binning parameters. Values on the vertical scale are the confidence levels for line detection. This is a very non-linear scale, with units in “number of nines”: i.e., levels of 0.9, 0.99, 0.999, etc. Mathematically, the “number of nines” is equal to $-\log_{10}(1 - P) - \log_{10}(N_{\text{chan}})$, where P is the probability of detection and the term with N_{chan} corrects the scale to account for the probability of a chance fluctuation given the number of channels in the spectrum. Without the channel number correction a “ 3σ ” excursion would be unremarkable: if drawn from normally distributed noise, one should appear every 370 samples, on average, and each confidence plot contains results from 52 different binnings, each with 50–200 channels, for a total of 9804 points. Regions where the columns coherently climb above 2 (0.99 confidence) give frequencies where a potential detection is insensitive to exact binning, indicating that the channel is reliably above or below the mean of its neighbors.

Vertical dashed lines through Figure 1 show the frequencies of the 1–0 lines measured from fits to the full-resolution unbinned 1–0 spectra of the two sources shown over small frequency ranges in Figures 2 and 3. Since the 1–0 and 3–2 redshifts agree to high precision, these also mark the 3–2 redshifts. An advantage of observing with a fixed-tuned broadband system is that it is possible to make direct comparisons of spectra and system performance for all sources. In all of the spectra we

Table 2

Summary of Results and Comparison to 3–2 Data from Downes & Solomon (2003) for SMM J14011+0252

Parameter	CO (1–0)	CO (3–2)
LSR redshift	2.5652 ± 0.0002	2.5652 ± 0.0001
Peak flux density, S_ν (mJy)	1.85 ± 0.20	13.2 ± 1
Line width (km s ⁻¹)	≤ 208	190 ± 11
Integrated line intensity (Jy km s ⁻¹)	~0.4 ± 0.05	2.8 ± 0.3
Integrated intensity ratio, $I(3-2)/I(1-0)$	6.6 ± 1.0	...
Integrated brightness temperature ratio, $R_{3,1}$	0.76 ± 0.12	...

Table 3

Summary of Results and Comparison to 3–2 Data from Weiß et al. (2009a) for SMM J14009+0252

Parameter	CO (1–0)	CO (3–2)
LSR redshift	2.9346	2.93450 ± 0.00035
Peak flux density, S_ν (mJy)	0.65	5.4 ± 0.9
Line width (km s ⁻¹)	643	470 ± 60
Integrated line intensity (Jy km s ⁻¹)	0.44	2.7 ± 0.3
Integrated intensity ratio, $I(3-2)/I(1-0)$	6.1 ± 0.7	...
Integrated brightness temperature ratio, $R_{3,1}$	0.67 ± 0.08	...

Notes. Structure in the spectral baseline rendered the line fits too poor for believable error estimates, so we quote the best fit without errors for linewidth and peak intensity. Integrated intensity ratios and errors are derived from a bootstrap analysis; see the text.

have taken with the Zpectrometer, there have been no signs of spurious detections, and specifically none at frequencies corresponding to either of these sources.

The smooth lines in Figures 2 and 3 represent simple Gaussian profile interpretations of the 3–2 line parameters. Tables 2 and 3 give the fit parameters and compare them with the 3–2 parameters from the literature. At the Zpectrometer’s maximum frequency resolution, spectral structure is correlated over about three bins; we correct for that in linewidth measurements.

For SMM J14011+0252, both the figure and the tabulated data show that the agreement between the 1–0 and 3–2 redshifts is excellent, and that the linewidths are very similar (3–2 data from Downes & Solomon 2003, which agrees well with Frayer et al. 1999). The integrated line intensity in Table 2 is from the Gaussian fit parameters to the line, with the 3–2/1–0 integrated intensity ratio equal to 6.8. Individual velocity-integrated flux densities (in this paper, the “integrated” in integrated intensities and brightness temperatures implies integration over the full linewidth in velocity) are computed from the fit parameters for a Gaussian profile, $\int S_\nu dv = 1.06 S_{\nu, \text{peak}} \Delta v_{\text{FWHM}}$.

More revealing than the flux density ratio is the integrated $J = 1-0$ and 3–2 brightness temperature ratio,

$$R_{3,1} = \frac{\int T(3-2) dv}{\int T(1-0) dv} = \frac{\int S_\nu(3-2) dv}{\int S_\nu(1-0) dv} \left(\frac{\nu_{1-0}}{\nu_{3-2}} \right)^2, \quad (1)$$

where $S_\nu(x - y)$ is the flux density in the $J = x - y$ transition and ν_{x-y} is the frequency of the transition. Departures of this ratio from unity reveal the departure from thick and thermalized emission from gas in the Rayleigh–Jeans limit. For this galaxy $R_{3,1} = 0.76$, lower than the value of unity expected in this single thick and thermalized limit. Errors in Table 2 and following tables are at the 68.3% (1σ equivalent for a normal distribution) confidence level for the fits, as determined by the R language’s `confint` routine.

SMM J14009+0252’s line is clearly detected when the binning concentrates most of the flux into one channel (Figure 1), but nonideal structure in the baseline hinders precise line amplitude and width measurements from full-resolution spectra.

Formal error estimates are consequently not realistic. Judging from the structure in Figure 3, the ripple in the spectrum causes the fit to underestimate the true 1–0 intensity and overestimate the linewidth; an integrated intensity estimate from the fit parameters is questionable. Instead, we derive the integrated intensity and errors from a bootstrap analysis of the numerator of Equation (A2) for the binning that yields the highest signal-to-noise detection, multiplying by a factor to account for flux outside the rectangular bin for a Gaussian lineshape. With 3–2 data from Weiß et al. (2009a), the 3–2/1–0 intensity ratio is 6.1, or $R_{3,1} = 0.67$.

3.2. SMM J04431+0210 and SMM J04433+0210

Figure 4 indicates that the only detection in this pair is of SMM J04431+0210; none of the negative-going structure is detected with high significance. The spectrum in the upper panel is binned for the best signal to noise for this line. The vertical dashed line is the measured 1–0 line frequency from a fit to the full-resolution 1–0 spectrum (Figure 5). Since agreement between the 1–0 and 3–2 redshifts are excellent, it could equally well indicate the 3–2 redshift. Figure 5 is a full-resolution spectrum, with the solid curve a single-component Gaussian profile fit. The dotted line represents the 3–2 line’s triangular shape (Neri et al. 2003), scaled to the 1–0 frequency, with the amplitude divided by 9. Lineshape differences between the two transitions are not large and could be due to noise in either spectrum or to physical substructure with somewhat different excitation conditions. Table 4 makes a numerical comparison between the 1–0 and 3–2 (Neri et al. 2003) line parameters, with the 1–0 parameters taken from the Gaussian profile fit. Taking the 3–2 integrated intensity from Neri et al. (2003), the 3–2/1–0 flux-density intensity ratio is 5.5 and $R_{3,1} = 0.61$.

The nondetection of SMM J04433+0210 could be due either to a redshift outside the Zpectrometer’s coverage ($2.2 \leq z \leq 3.5$ for CO 1–0, $5.4 \leq z \leq 8.0$ for CO 2–1) or to a low CO flux. The source has no known redshift, largely because its faint optical counterpart is challenging for spectroscopy ($K = 22.4$; Frayer et al. 2004), although the existence of a radio counterpart

Table 4
Summary of Results and Comparison to 3–2 Data from Neri et al. (2003) for SMM J04431+0210

Parameter	CO (1–0)	CO (3–2)
LSR redshift	2.5086 ± 0.0007	2.5094 ± 0.0002
Peak flux density, S_ν (mJy)	0.58 ± 0.08	3.5
Line width (km s^{-1})	415 ± 62	350 ± 60
Integrated line intensity (Jy km s^{-1})	0.26 ± 0.05	1.4 ± 0.2
Integrated intensity ratio, $I(3-2)/I(1-0)$	5.5 ± 1.4	...
Integrated brightness temperature ratio, $R_{3,1}$	0.61 ± 0.15	...

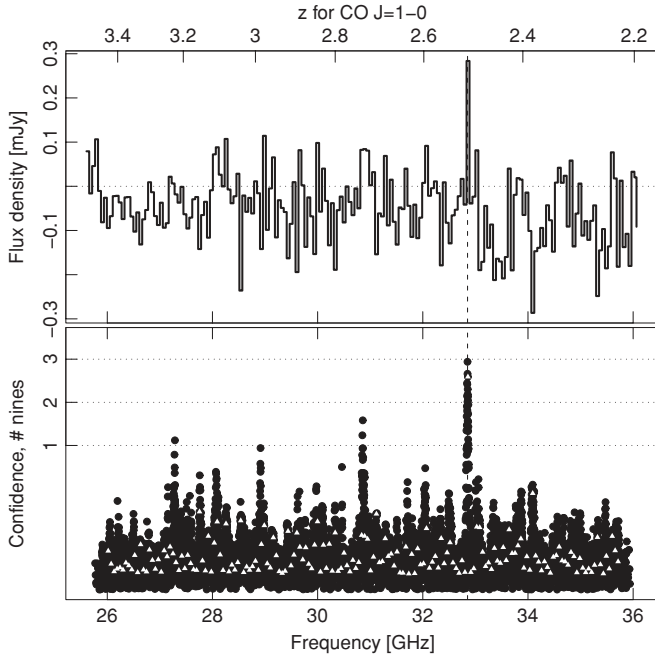


Figure 4. Difference spectrum of SMM J04431+0210 and SMM J04433+0210 (upper panel) and confidence plot (lower panel). The triangles in the confidence plot mark the points corresponding to the binning for the spectrum in the top panel. See the caption of Figure 1 for an explanation of the confidence scale.

suggests that it does not lie at a much higher redshift than the $z \sim 2.5$ radio-preselected SMGs of the Chapman et al. (2005) sample. Given that SMM J04433+0210’s $850 \mu\text{m}$ flux density of only 4.5 ± 1.5 mJy is barely above the detection threshold of the SLS (Smail et al. 2002), within the range where noise fluctuations can boost a weak detection significantly, we view low CO flux as the most likely reason for its nondetection.

4. DISCUSSION

We detected CO $J = 1-0$ emission from the three sources in our samples that have known CO 3–2 line parameters. The similarities of line redshifts and velocity widths for the 1–0 and 3–2 lines justify a joint analysis of the two. For the sample given in Section 2, the mean and standard deviation of the means is $R_{3,1} = 0.68 \pm 0.08$. Compared with other SMGs, the mean ratio from our sample is slightly higher than the ratio $R_{3,1} = 0.48$ for SMM J02399–0136 (Ivison et al. 2010a), the brightest of the SLS galaxies in $850 \mu\text{m}$ continuum, and is comparable to the ratio for the highly lensed SMG SMM J2135–0102, $R_{3,1} = 0.68$ (Swinbank et al. 2010; Danielson et al. 2010). For this sample of five SMGs with currently known 1–0 and 3–2 fluxes, the ratio is $R_{3,1} = 0.64 \pm 0.10$.

A sample of five is not large, but neither is it so small that a few additional observations can dramatically change the result. For example, if the ratio for most SMGs is really $R_{3,1} = 1$

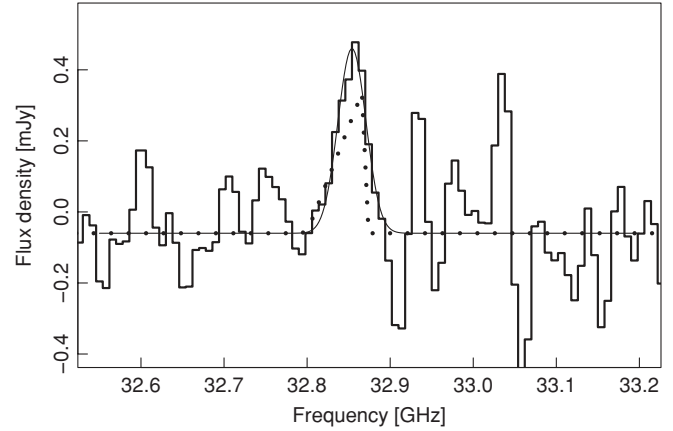


Figure 5. Spectrum of SMM J04431+0210 with Gaussian profile fit (curve) and triangular approximation to the 3–2 spectral lineshape with flux density divided by nine (dotted; Neri et al. 2003)

and we have been unlucky in our choice of galaxies, it will take observations of another 13 galaxies with unity ratio to reach a sample mean ratio of $R_{3,1} = 0.9$. Roughly speaking, observations of 15 additional galaxies will be needed to reduce the dispersion by a factor of two. We can also estimate the chances that we have drawn five of five galaxies with $R_{3,1}$ below the true mean. From the binomial theorem, the probability is 0.03, for a symmetrical distribution where each draw has a probability 0.5 of being above or below the mean. These simple considerations indicate that our conclusion that $R_{3,1} \approx 0.6$ in SMGs is robust. A recent independent data set based on EVLA data gives $R_{3,1} \approx 0.55$ (R. J. Ivison 2010, private communication; Ivison et al. 2010b), in agreement with our value within errors.

The values of mean and dispersion in $R_{3,1}$ carry two linked implications: the first one for mass estimates that rely on line luminosity scaling and the second for the state of the typical interstellar medium (ISM) in SMGs.

Observers have had to use incomplete data along with assumptions and approximations to make mass estimates for distant galaxies. In mass derivations from millimeter wave spectroscopy of SMGs, which are most often observed in the mid- J lines, a frequent implicit assumption is that the CO lines share the same excitation temperature T_{ex} from the observed mid- J transition down to the 1–0 line at the base of the CO rotational ladder. An alternative to the assumption of constant T_{ex} has been to fit observed line fluxes to a single-component ISM radiative transfer model (e.g., Weiss et al. 2007) and then use the model predictions for unobserved line fluxes. The CO 1–0 data we report probe the ground-state emission of the CO molecule to provide critical tests for these assumptions, which of necessity invoke simple interstellar media.

The excitation temperature, T_{ex} , is a very general concept that describes an energy density, whether kinetic, radiative,

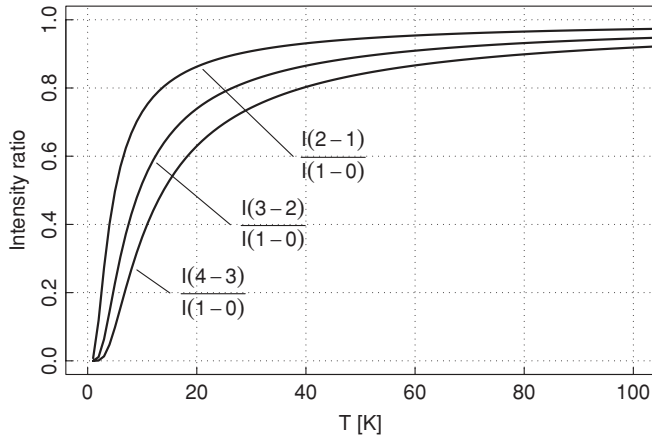


Figure 6. Values of Planck function ratios for optically thick and thermalized gas for $J \leq 4$. The ratios reach the Rayleigh–Jeans limit, in which the radiation and kinetic temperatures are approximately equal, when the frequency ν of the higher frequency line is $h\nu/k \gg T$.

rotational, vibrational, spin, etc. In observational molecular spectroscopy T_{ex} is the measured quantity; for the rotational transitions of the CO molecule, the excitation temperature is the rotational temperature T_{rot} . In this paper, we use the term thermalized in its rigorous sense, to mean that T_{rot} is equal for all transitions of interest. Thermalized in this sense does not necessarily imply that the molecule is in local thermodynamic equilibrium, with rotational temperature equal to the kinetic temperature of the surrounding H_2 molecules, although this is often the case for low- J CO transitions and is a common use of the term. In a rigorous context, the term subthermal indicates that the excitation temperature T_{rot} for a given transition is below T_{rot} of a comparison transition from the same ensemble of molecules, without reference to T_{kin} , T_{rad} , or any other external bath.

Strictly speaking, the usual practice of extrapolating a constant radiation temperature T_{rad} measured in a mid- J line for lower- J transitions is incorrect even if the density is high enough that $T_{\text{rot}} = T_{\text{kin}}$: the kinetic temperature in SMGs is unlikely to be high enough to drive T_{rad} into the asymptotic Rayleigh–Jeans limit. As Figure 6 illustrates, the Planck radiation (brightness) temperature ratios for even low- J lines still climb toward unity for $T < 100$ K, so $I_\nu \propto T_{\text{rad}} \neq T_{\text{kin}}$. At a typical SMG dust temperature of about 40 K (Blain et al. 2002) the correction from the Rayleigh–Jeans limit is a factor of 1.2 for the 4–3 line, with corrections increasing with J . If uncorrected, errors from the Rayleigh–Jeans approximation add artificial rolloff to plots of CO line intensity versus J when those plots involve scaling intensity by frequency squared to find the collapse of excitation with J .

Returning to the observations, the small dispersion in $R_{3,1}$ justifies an empirical scaling prescription between the two intensities for many sources, although there will doubtless be excursions far from the mean for individual sources where scaling fails. In the local universe, an integrated brightness temperature of the CO 1–0 line, $I_{\text{CO}} = \int T_{1-0} d\nu$, has been used extensively to estimate total molecular gas column densities. The 1–0 transition traces molecular gas with a wide range of excitation and is relatively easy to observe in nearby sources. Although optically thick, it can trace mass by “cloud-counting” many individual clumps at different velocities within a telescope’s beam (e.g., Dickman et al. 1986). Integrating I_{CO} over projected area defines a luminosity L'_{CO} that is directly proportional to molecular

gas mass; Solomon et al. (1992) derive a form appropriate at cosmological distances as $L'_{\text{CO}} = I_{\text{CO}} \Omega_s D_A^2$, where Ω_s is the source solid angle and angular diameter distance D_A accounts for cosmology. I_{CO} is related to the H_2 column density $N(\text{H}_2)$ through the X factor, and L'_{CO} to gas mass through the α factor. X and α differ by a constant factor and have been calibrated for the 1–0 line in Galactic, starburst, and ULIRG environments; Tacconi et al. (2008) provide a brief critical review of applying these scale factors in the high-redshift universe.

In the framework of scaling luminosity between different lines, the mean value of $R_{3,1} = 0.64$ we find shows that a scaling factor of about $1/0.64 = 1.5$ is likely to be a more accurate predictor of the 1–0 integrated intensity from the 3–2 integrated intensity than a factor of unity. To first order, this will increase gas masses deduced from assuming $L'_{\text{CO}1-0} = L'_{\text{CO}3-2}$ by a factor of 1.5.

Departures from a ratio of unity are not limited to the 3–2/1–0 pair. Finding values other than unity from actual 1–0 observations of SMGs is becoming commonplace. Hainline et al. (2006) and Carilli et al. (2010) found similar behavior in their 1–0 observations of SMM J13120+4242 and GN20, with an equivalent ratio $R_{4,1}$ of 0.26 (with some uncertainty from low-level emission in line wings) and 0.45, respectively. The deviations from a simple thick and thermalized model are in the same direction as we find, but are larger and the scatter in the ratio is much higher.

Many of the earlier explanations for the lack of equality in line brightness temperatures invoked subthermal (in the rigorous sense we discussed) excitation of the mid- J lines in such a simple, single-component ISM as an explanation for decreasing T_{ex} with J . We do not agree with this approach because it is an unphysical distraction rather than a useful approximation. Multi-line observations of nearby galaxies (and, for that matter, Galactic giant molecular clouds) show interstellar media with multiple components as defined by lineshape, emission from different molecular species, or detailed physical conditions. If the 1–0 and 3–2 emission in the SMGs we observe were from a single component of subthermally excited gas, the 3–2 intensity would be very sensitive to the detailed physical conditions. We modified an escape-probability radiative transfer code (J. Stutzki 2005, private communication; Stutzki & Winnewisser 1985; cross-sections from Flower & Launay 1985) to explore conditions matching a conservatively broad range of $R_{3,1} = 0.6 \pm 0.2$. To ensure our model produced reasonable emissivities, we eliminated solutions with optical depths less than unity in both lines. The formal solutions are in Figure 7. Solutions with densities much above 10^3 cm^{-3} are not likely to be of physical importance. First, the high-density solutions occur at low temperatures, where the lines are extremely weak since they are close to the $T = 9.6$ K background temperature at the model’s $z = 2.5$. Such lines will not dominate the molecular gas luminosity. Further, it is questionable whether the bulk of high-density gas could be much colder than the bulk of the dust, which has a temperature of about 40 K in SMGs (Blain et al. 2002). Overall, the model indicates that subthermally excited gas would have a density of a few $\times 10^2 \text{ cm}^{-3}$ at a CO column density of $5 \times 10^{18} \text{ cm}^{-2}$ in a 400 km s^{-1} linewidth, with lower densities possible at higher columns.

Explanations for line ratios that require very specific physical conditions (or a very constant gravitational lens amplification ratio for the two lines) are not supported by the low dispersion of $R_{3,1}$ from even our handful of SMGs. It is unrealistic to expect such a tight range of parameters from sample of galaxies selected

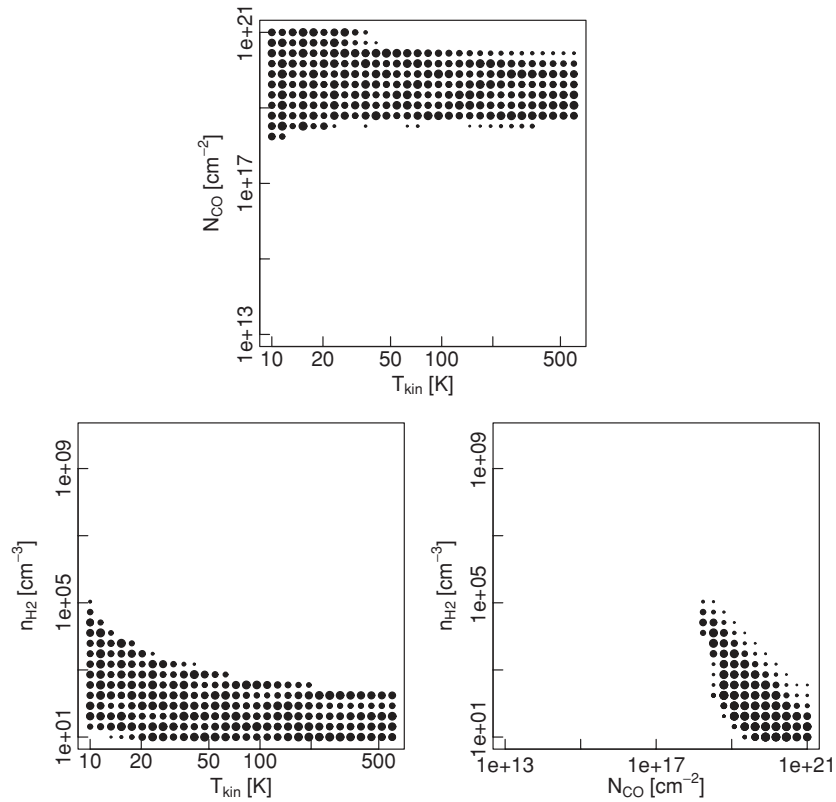


Figure 7. Side views of the three-dimensional volume containing radiative transfer calculation results to identify the physical conditions that produce $R_{3,1} = 0.6 \pm 0.2$ by subthermal excitation. The plot is a summary of 27k models filling the volume with equal spacing as seen in the projected views. The points represent successful models, with size corresponding to the ratio: the largest diameter points are near the observed ratio of $R_{3,1} = 0.6$ and the smallest at $R_{3,1} = 0.4$ and 0.8 . Results for optically thin lines have been removed from this summary to satisfy observational constraints. High-density, low-temperature results are not likely to be physical; see the text.

without regard for their CO emission properties, especially so when observations of other lines directly contradict the special conditions. Interstellar media dominated by low-density material are incompatible with detections of CO $J = 7-6$ from SMM J14011+0252 (Downes & Solomon 2003), and $J = 5-4$ from SMM J14009+0252 (Weiß et al. 2009a); these lines are strong and rule out CO excitation that is collapsing by $J = 3$. The presence of excited gas in these sources does not seem to be unusual: a compendium of CO excitation diagrams in Weiss et al. (2007) shows that the brightest CO lines are in states J of 5–6 for typical SMGs.

Brightness temperature ratios $R_{3,1} < 1$ are not peculiar to SMGs, but are common in most galaxies. Yao et al. (2003) and Mauersberger et al. (1999) report mean values of $R_{3,1} = 0.66$ and $R_{3,1} = 0.63$, respectively, in different samples of luminous galaxies in the local universe. Iono et al. (2009) find a mean $R_{3,1} = 0.48$ for dusty U/LIRGs at an altogether different redshift, and Aravena et al. (2010) find $R_{3,1} = 0.61$ for a $z = 1.5$ BzK galaxy selected by its rest-UV/optical colors. At the same time, Bayet et al. (2006) find that CO ladder excitation peaks at $J \sim 4$ for the Galaxy and IC 342, and at $J \sim 7$ for starbursts, a type common in the Yao et al. (2003) and Mauersberger et al. (1999) samples. The excitation rolloff seems to shift to much higher J for very luminous active galactic nucleus hosts: Van der Werf et al. (2010) find that $J = 13-12$ is still strong in the ULIRG Mrk 231, and Bradford et al. (2009) find strong lines to $J = 9$ in the Cloverleaf QSO.

A pattern of apparently subthermal line ratios from an ISM that also has strong emission from lines at higher J is a clear signature of a multi-component ISM. In any given line from an

ISM with a range of physical conditions, the warmest optically thick regions with the largest area filling factors will dominate the emission. Basic excitation considerations suggest strong 1–0 emission from distributed gas, while the 3–2 emission is dominated by star forming and other regions with enhanced excitation. High-spatial resolution observations of SMGs do show varying size with excitation. Danielson et al. (2010) find systematic lineshape and size changes with J in CO emission toward one source. Bothwell et al. (2010) show that mid- J CO emission regions’ sizes are different than the sizes of the star formation as traced by radio continuum. R. J. Ivison (2010, private communication; Ivison et al. 2010b) make a comparison of emission sizes in the CO 1–0 and mid- J transitions. Evidence for higher excitation in the centers of local U/LIRGs (Iono et al. 2009), which numerical models imply may also characterize high-redshift SMGs (Narayanan et al. 2009), suggests that the balance between components is partly set on galaxy-wide scales. Narayanan et al. (2009) run hydrodynamic simulations of galaxy mergers that yield SMG luminosities, finding that the resulting ISM produces galaxy-averaged CO emission with line ratios that mimic subthermal excitation from a single-component ISM. While this qualitatively matches the data, the observed 3–2/1–0 flux ratio of 5.8 ± 0.9 is higher than the model results of 3 ± 1 , indicating that the gas is somewhat more excited than predicted. Bringing the model results into better agreement with observations may be useful in refining modeling prescriptions. Overall, given the wide range of galaxies that show a similar $R_{3,1}$ and lack of correlation with most physical properties that Yao et al. (2003) find for $R_{3,1}$, it is plausible that the different lines trace different mixtures of regions in an ISM with a hierarchical

(e.g., self-similar, fractal) geometry, as is commonly found in high resolution observations of our Galaxy and emerges from numerical simulations of cloud structure.

At this stage we do not have enough lines to identify ISM structures or to separate components through radiative transfer calculations, but we can draw some simple conclusions from basic considerations. The brightnesses of the lines and correlation between 1–0 and 3–2 intensities indicate that the individual lines are optically thick. Deviations from $R_{3,1} = 1$ then come from different geometrical filling factors of related components in a multi-component ISM, with a small contribution from failure to reach the asymptotic Rayleigh–Jeans limit (Figure 6).

Finding a multi-component ISM in SMGs has implications for the choice of relationship between CO 1–0 intensity and mass, $M = \alpha L'_{\text{CO}}$. The value used most often for SMGs is $\alpha = 0.8 (M_{\odot} \text{ km s}^{-1} \text{ pc}^2)^{-1}$ (reviewed with caveats in Solomon & Vanden Bout 2005), which was derived for ULIRGs from radiative transfer calculations based on an interpretation of a 2–1/1–0 integrated brightness temperature ratio below one as evidence of subthermal excitation in ULIRGs (Downes & Solomon 1998). An ISM similar to other galaxies favors values for α closer to calibrations from the dense parts of starburst nuclei or the Galaxy (see Tacconi et al. 2008 for a summary and references to individual studies). Compounding the factor of $(R_{3,1})^{-1} = 1.5$, an increase in α by a factor of about 2 would increase mass estimates for the SMGs by an overall factor of about 3. Increased mass estimates also imply decreased star formation efficiency estimates. Large masses derived from scaling factors will run into upper limits set by dynamical mass measurements and may indicate that the local (Galactic) [CO]/[H₂] abundance ratio is lower than those in high-redshift SMGs.

In summary, we find observationally that a luminosity ratio of $L'_{\text{CO}}(3-2) \approx 0.6 \times L'_{\text{CO}}(1-0)$ is more appropriate than the customary assumption of equality. Scaling the 3–2 integrated brightness temperatures to 1–0 does seem to be empirically justified, but a factor of $0.64^{-1} = 1.5$ is more appropriate than unity. Increasing the scaling factors for both line integrated intensities and the conversion between line luminosity and mass, as suggested by the similarity of $R_{3,1}$ in SMGs and local luminous galaxies, would increase mass estimates from observed 3–2 lines for SMGs further, unless conversion factors are allowed to change with environment. Increasing the scaling factor would increase simple molecular mass estimates for SMGs and decrease their derived star formation efficiencies. It appears that simple line flux scaling breaks down beyond $J = 3$, as although the trend in the line ratios are similar, the dispersion in temperature ratios becomes substantially larger, probably because the higher- J lines probe past the average peak excitation. The large number of galaxies with similar $R_{3,1}$ ratios, SMGs included, indicates that single-component models are inadequate descriptions of what must be more complex interstellar media. Identifying galaxies with $R_{3,1}$ considerably different from the typical value of 0.6 will be valuable in understanding the origin of the typical conditions in the ISM.

This material is based on work supported by the National Science Foundation under grant numbers AST-0503946 to the University of Maryland and AST-0708653 to Rutgers University. We thank the NRAO staff, particularly P. Jewell, R. Prestage, K. O’Neil, R. Maddalena, B. Mason, A. Shelton, R. Norrod, and the GBT software, mechanical design, and operations groups for their support and contributions. We thank J. Stutzki for a

copy of his radiative transfer code, A. Bolatto, D. Frayer, E. Ostriker, and R. Shetty for perceptive comments, A. Weiß for confirming our first estimate of J14009+0252’s redshift before publication of his data, and L. Hainline for her contribution to the data reduction software and for critical comments on the paper. The National Radio Astronomy Observatory is a facility of the National Science Foundation operated under cooperative agreement by Associated Universities, Inc.

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APPENDIX

LINE DETECTION CONFIDENCE METHOD

Our detection confidence calculation is based on determining whether a channel has a systematically different amplitude from its neighbors. Setting a detection criterion for the line amplitude in a single channel would be simple if we somehow knew the mean value with no line present and had accurate knowledge of the system fluctuation within the channel. However, typical broadband spectra have offsets and other large-scale structures in the spectral baseline, and the noise may change with frequency as the receiver or system temperatures change. Estimating noise parameters by calculating, for instance, the standard deviation across frequency channels will be misleading in such cases. Comparing the mean value of a channel with those of its neighbors is more fruitful, as neighbors are likely to share offsets and noise. Limiting the number of neighbors increases the uncertainty of noise estimates in the spectral domain, however. The time sequence of data within each channel, sampled by the many subs cans in a long integration, provides information on the fluctuations in each channel.

Our detection calculation is based on comparing mean values between neighboring frequency channels, using noise estimates derived from the time sequences of individual channels to calculate the statistical significance of departures from the mean, with detection significance framed in a classical hypothesis test. Rather than testing for a detection of a line with unknown amplitude, we find the probability that the null case of no detection fails. If a spectral line is *not* present in the parent data, then the mean value in some channel X will be equal to the mean value of its M neighbors Y_i :

$$\bar{X} - \frac{1}{M} \sum_{i=1}^M \bar{Y}_i = 0 \quad (\text{A1})$$

within fluctuations from noise.

To estimate the fluctuation in each channel, we calculate sample variances S_X^2 and $S_{Y_i}^2$ in the time sequence of each channel, derived from the N 4 minute subs cans in our final spectra. This approach provides estimates for individual channels, independent of systematic structure across the spectrum.

Combining the difference in means and channel amplitude uncertainties, a suitable test statistic is

$$d = \frac{(\bar{X} - \frac{1}{M} \sum_{i=1}^M \bar{Y}_i)}{\sqrt{\frac{1}{NM} (S_X^2 + \sum_{i=1}^M S_{Y_i}^2)}} \quad (\text{A2})$$

This is a useful form because it has a Student- t distribution with $(M + 1)(N - 1)$ degrees of freedom in the case that the signals in all channels X and Y_i are from the same normally distributed parent population. While this condition cannot be strictly true in general, it can be a quick and reasonable

approximation for channels close together in frequency and over times short compared with atmospheric changes; t -tests tend to be robust. As values of d become far from zero, the value produced by a nondetection, it becomes less likely that the true value is zero within fluctuations, and more likely that a real deviation from a mean value of zero has been detected. For an emission line search, where even a large negative excursion counts as a nondetection, the probability that the measured weighted difference d is consistent with zero is the one-tailed test:

$$P(\text{fluctuation} \geq d) = P(d \geq t_{\alpha, (M+1)(N-1)}) \\ = \int_d^{\infty} T_{(M+1)(N-1)}(u) du. \quad (\text{A3})$$

In searching for positive and negative excursions, as we would with our difference spectra, a two-tailed test is appropriate.

In practice, absolute probabilities given by Equation (A3) are approximate because the assumptions of stationary statistics with equal variances for all neighbors are not strictly correct. In addition, this analytical approach has no way to accommodate weighting (e.g., for changes of atmospheric transmission with time) during data analysis. To counter these shortcomings, we turned to the bootstrap technique (see Efron & Tibshirani 1994), creating bootstrapped spectra by randomly drawing the same number of subscans as in the initial data set, with replacement (duplicates are allowed), from the pool of subscans. The bootstrapped spectra can then be suitably weighted averages of individual subscans. For the examples in this paper, we made 2000 bootstrapped spectra for each source pair, or 2000 examples of spectra we might have observed assuming the pool of subscans is representative of all data (this is the fundamental principle behind the bootstrap). We then used Equation (A2) as the “studentized” detection statistic, since eliminating scale gives pivotal (variance stabilized) forms with superior properties in bootstrap confidence calculations (Efron & Tibshirani 1994; Zoubir & Iskander 2004). The resulting distribution of d should be very closely normal, with the central limit theorem acting on sums of the nearly normal statistic d . We verified the assumption by comparing the distributions of d and the normal distribution on quartile–quartile plots, finding that the probabilities determined by counting bootstrap results and by the normal approximation were the same within fluctuations from finite sample length.

Counting bootstrapped results that satisfy a condition and then normalizing by the number of bootstrap samples gives distribution-independent probability estimates, with the probability range bounded by the number of samples. Samples of 2000 are suitable for finding distribution-independent probabilities to about 0.99, for instance. To increase the confidence limit range we could have either increased the number of bootstrap samples or used the empirical agreement of the studentized d to the normal distribution. We chose the latter as a conservative approximation: the observed bootstrap result distribution should be, and empirically is, closely normal; because a normal approximation is insensitive to a few extreme results and because of practical limits on computational time. Even with the calculation of d in a compiled code function to speed iterative calculations within the R language framework we use, typical run times for a full range of binning were about a minute, so increasing the number of samples by a few orders of magnitude from 2000 was impractical for interactive analysis.

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