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The ALMA-PILS survey: First detections of ethylene oxide, acetone and propanal toward the low-mass protostar IRAS 16293-2422

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ABSTRACT

Context. One of the open questions in astrochemistry is how complex organic and prebiotic molecules are formed. The unsurpassed sensitivity of the Atacama Large Millimeter/submillimeter Array (ALMA) takes the quest for discovering molecules in the warm and dense gas surrounding young stars to the next level.

Aims. Our aim is to start the process of compiling an inventory of oxygen-bearing complex organic molecules toward the solar-type Class 0 protostellar binary IRAS 16293-2422 from an unbiased spectral survey with ALMA, Protostellar Interferometric Line Survey (PILS). Here we focus on the new detections of ethylene oxide (c-C₂H₄O), acetone (CH₃COCH₃), and propanal (C₂H₅CHO).

Methods. With ALMA, we surveyed the spectral range from 329 to 363 GHz at 0.5'' (60 AU diameter) resolution. Using a simple model for the molecular emission in local thermodynamical equilibrium, the excitation temperatures and column densities of each species were constrained.

Results. We successfully detect propanal (44 lines), ethylene oxide (20 lines) and acetone (186 lines) toward one component of the protostellar binary, IRAS 16293B. The high resolution maps demonstrate that the emission for all investigated species originates from the compact central region close to the protostar. This, along with a derived common excitation temperature of $T_{\text{ex}} \approx 125$ K, is consistent with a coexistence of these molecules in the same gas.

Conclusions. The observations mark the first detections of acetone, propanal and ethylene oxide toward a low-mass protostar. The relative abundance ratios of the two sets of isomers, a CH₃COCH₃/C₂H₅CHO ratio of 8 and a CH₃CHO/c-C₂H₄O ratio of 12, are comparable to previous observations toward high-mass protostars. The majority of observed abundance ratios from these results as well as those measured toward high-mass protostars are up to an order of magnitude above the predictions from chemical models. This may reflect either missing reactions or uncertain rates in the chemical networks. The physical conditions, such as temperatures or densities, used in the models, may not be applicable to solar-type protostars either.

Key words. astrochemistry – ISM: molecules – ISM: abundances – ISM: individual object: IRAS 16293-2422
line: identification – astrobiology

1. Introduction

An important task of modern-day astrochemistry is to understand how complex organics and possible pre-biotic molecules form near young stars. The high sensitivity and angular and spectral resolution of the Atacama Large Millimeter/submillimeter Array (ALMA) enables detection of molecular species with faint emission lines in otherwise confused regions. The capabilities of ALMA were demonstrated early on by the first detection

of the prebiotic molecule glycolaldehyde toward the low-mass protostar, IRAS 16293-2422 (Jørgensen et al. 2012). This detection illustrates the potential for imaging emission from the simplest building blocks for biologically relevant molecules during the earliest stages of the Solar System on the scales where protoplanetary disks emerge, and for understanding how these molecules are formed and in what abundances. This paper presents the first detections of three such species, ethylene oxide (c-C₂H₄O), propanal (C₂H₅CHO) and acetone (CH₃COCH₃)

toward IRAS 16293-2422 from an unbiased spectral survey with ALMA (Protostellar Interferometric Line Survey or PILS; Jørgensen et al. 2016).

Traditionally, detections of complex organic molecules have mostly been associated with the hot cores around high-mass protostars toward the warm and dense central regions around such luminous sources where the molecules sublimate from the icy mantles of dust grains. Some low-mass protostars show similar characteristics on small scales; the so-called *hot corinos* (van Dishoeck & Blake 1998; Bottinelli et al. 2004; Ceccarelli 2004). A prime example of this is IRAS 16293-2422 (IRAS 16293 hereafter), a protostellar Class 0 binary system, located at a distance of 120 pc (Loinard et al. 2008). IRAS 16293 is perhaps the best low-mass protostellar testbed for astrochemical studies (see, e.g., Blake et al. 1994; van Dishoeck et al. 1995; Ceccarelli et al. 2000; Schöier et al. 2002). It has the brightest lines by far of all well-studied low-mass protostars and shows detections of a wealth of complex organic molecules (Cazaux et al. 2003; Caux et al. 2011). These complex organics arise in the dense gas around each of its two binary components that each show distinct chemical signatures in the warm gas on small scales resolved by (sub)millimeter wavelength aperture synthesis observations (Bottinelli et al. 2004; Kuan et al. 2004; Bisschop et al. 2008; Jørgensen et al. 2011).

To understand how these complex organic molecules form, combinations of systematic studies establishing large inventories of similar organic molecules are needed. For this purpose, structural isomers are particularly interesting since they usually share some formation and destruction pathways. The relative abundance of two such isomers may therefore provide important constraints on astrochemical models. Examples of such interesting isotope pairs are ethylene oxide and acetaldehyde as well as acetone and propanal. Ethylene oxide was first detected toward the galactic center source Sagittarius B2(N) (Sgr B2(N)) by Dickens et al. (1997; confirmed by Belloche et al. 2013), and has since been observed in several massive star-forming regions (Nummelin et al. 1998; Ikeda et al. 2001) but so far not toward any low-mass protostar. Acetone (CH_3COCH_3), also called propanone, was the first molecule with ten atoms to be observed in the ISM. The molecule was first detected in the hot molecular core Sgr B2 (Combes et al. 1987; Snyder et al. 2002) and later in the Orion-KL star-forming region (Friedel et al. 2005; Friedel & Snyder 2008; Peng et al. 2013). It was also detected toward other massive star-forming regions (Isokoski et al. 2013) as well as toward an intermediate-mass protostar (Fuente et al. 2014). Several lines of the SMA survey of IRAS 16293 were also assigned to acetone by Jørgensen et al. (2011), but it has never been properly identified in this source. More recently, it was found in material from the comet 67P/Churyumov-Gerasimenko by the COMetary Sampling And Composition (COSAC) experiment on Rosetta’s lander Philae (Goesmann et al. 2015). Propanal ($\text{C}_2\text{H}_5\text{CHO}$) has previously been detected in Sgr B2(N) by Hollis et al. (2004), where it coexists with propynal and propenal. It was also detected towards two Galactic center molecular clouds by Requena-Torres et al. (2008). Like acetone, propanal was found to be present in the comet 67P/Churyumov-Gerasimenko (Goesmann et al. 2015).

This paper presents detections of ethylene oxide, acetone and propanal toward IRAS 16293 utilising a large ALMA survey at (sub)millimeter wavelength. These are all first time detections in IRAS 16293 and in low-mass protostars in general. In Sect. 2, we briefly describe the observations. The identification and analysis of the data are presented in Sect. 3. Finally, we discuss the results in Sect. 4 and conclude in Sect. 5.

2. Observations

IRAS 16293 was observed as part of the PILS program (PI: Jes K. Jørgensen): the survey consists of an unbiased spectral survey covering a significant part of ALMA’s Band 7 (wavelengths of approximately 0.8 mm) as well as selected windows in ALMA’s Bands 3 (at approximately 100 GHz; 3 mm) and 6 (at approximately 230 GHz; 1.3 mm). In this paper we only utilise data from the Band 7 part of the survey (project-id: 2013.1.00278.S). An observing log, a description of the data reduction and a first overview of the data are presented in Jørgensen et al. (2016) and here we only summarize a number of the key features of the Band 7 observations.

The Band 7 part of the survey covers the frequency range from 329.15 GHz to 362.90 GHz in full. Data were obtained from both the array of 12 m dishes (typically 35–40 antenna in the array at the time of observations) and the Atacama Compact Array (ACA), or “Morita Array”, of 7 m dishes (typically 9–10 antenna in use). The pointing center was in both cases set to be a location in-between the two components of the binary system at $\alpha_{J2000} = 16^{\text{h}}32^{\text{m}}22.72^{\text{s}}$; $\delta_{J2000} = -24^{\circ}28'34''.3$. In total 18 spectral settings were observed: each setting covers a bandwidth of 1875 MHz (over four different spectral windows of 468.75 MHz wide). To limit the data-rate, the data were downsampled by a factor two to the native spectral resolution of the ALMA correlator, resulting in a spectral resolution of 0.244 MHz ($\approx 0.2 \text{ km s}^{-1}$) over 1920 channels for each spectral window. Each setting was observed with approximately 13 min integration on source (execution blocks of approximately 40 min including calibrations) for the 12 m array and double that for the ACA.

The data for each setting were calibrated and a first imaging of the continuum was performed. Thereafter, a phase-only self-calibration was performed on the continuum images and applied to the full datacubes before combining the 12 m array and ACA data and performing the final cleaning and imaging. The resulting spectral line datacubes have a root mean square (RMS) noise for the combined datasets of approximately 6–8 mJy beam $^{-1}$ channel $^{-1}$, which translates into a uniform sensitivity better than 5 mJy beam $^{-1}$ km s $^{-1}$ with beam sizes ranging from ≈ 0.4 – $0.7''$ depending on the exact configuration at the date of observation. The data used in this paper were produced with a circular restoring beam of $0.5''$ to facilitate the analysis across the different spectral windows. The conversion from Rayleigh-Jeans temperature $T_{\text{b}}[\text{K}]$ to flux density $S_{\nu}[\text{Jy}/\text{beam}]$ follows the standard formulation and T_{b}/S_{ν} ranges from 37.2 to 45.2 KJy $^{-1}$ depending on the frequency. The resulting image cubes are strongly line-confused toward the locations of the two primary protostars. A subtraction of the continuum was therefore done statistically for each spectral window (for continuum maps and more details see Jørgensen et al. 2016). The continuum baseline for each window is found to be robust to within twice the RMS in each channel.

3. Analysis and results

Interferometric emission maps of two representative lines each for propanal, acetone, ethylene oxide, and acetaldehyde are shown in Fig. 1. The maps show emission toward both protostellar sources. Generally the lines toward IRAS 16293A are approximately a factor five broader than toward IRAS 16293B (e.g., Bottinelli et al. 2004; Jørgensen et al. 2011), which makes identification of individual species challenging. Consequently IRAS 16293B is therefore better for separation of blended lines

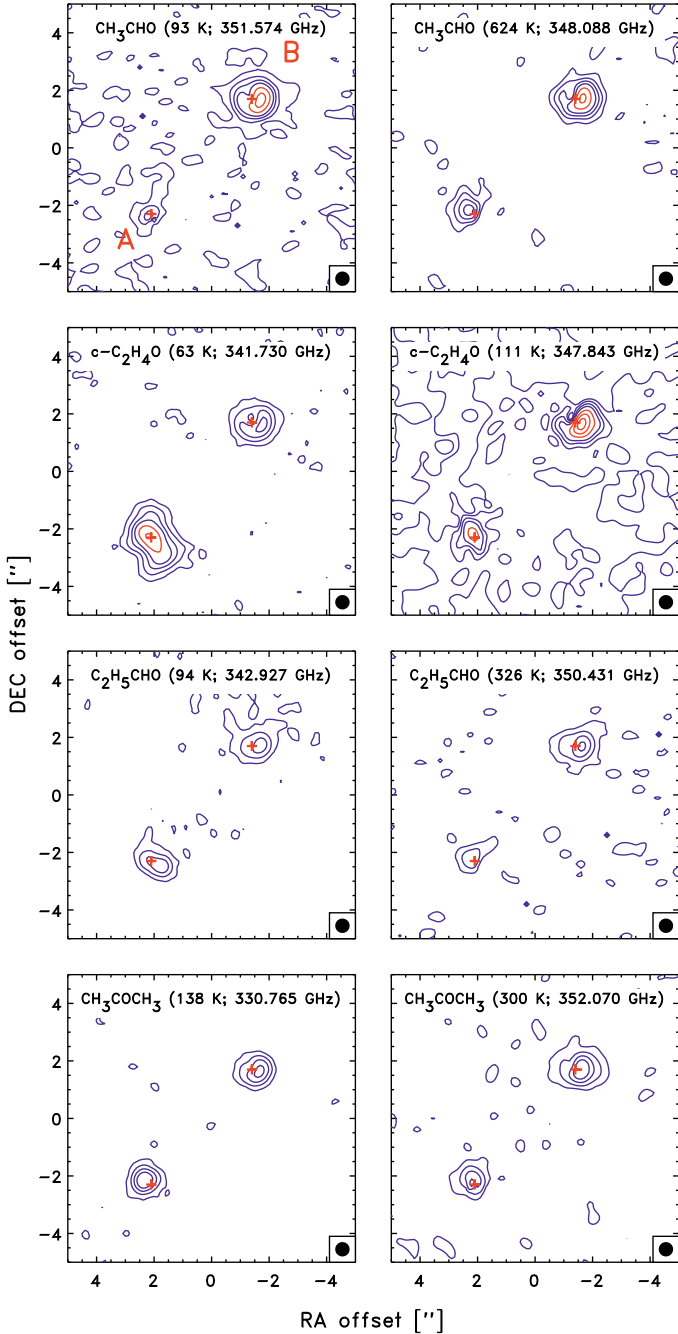


Fig. 1. Integrated intensity maps of the line emission for acetaldehyde, ethylene oxide, acetone, and propanal. *Left and right columns* show maps for transitions with lower and higher E_{up} , respectively. The locations of IRAS 16293A (southeast) and IRAS 16293B (northwest) are marked by the red plus-signs. The blue contours represent 4, 8, 12 and 16σ while the red contours show 24, 30, 36σ , where σ is $5 \text{ mJy beam}^{-1} \text{ km s}^{-1}$ for the integrated intensity. A representative beam of $0.5''$ is shown in the lower right-hand corner of each panel.

and identification of new species and in this paper we focus on that source. A comparison of the maps for the different molecules shows that the emission is marginally resolved toward IRAS 16293B, consistent with a deconvolved extent of $\approx 0.5''$ toward the location of the protostar for all species. We can therefore assume that these particular molecules coexist and trace the same gas. Extracting a spectrum from the pixel located on the peak position will give the highest emission signal, but

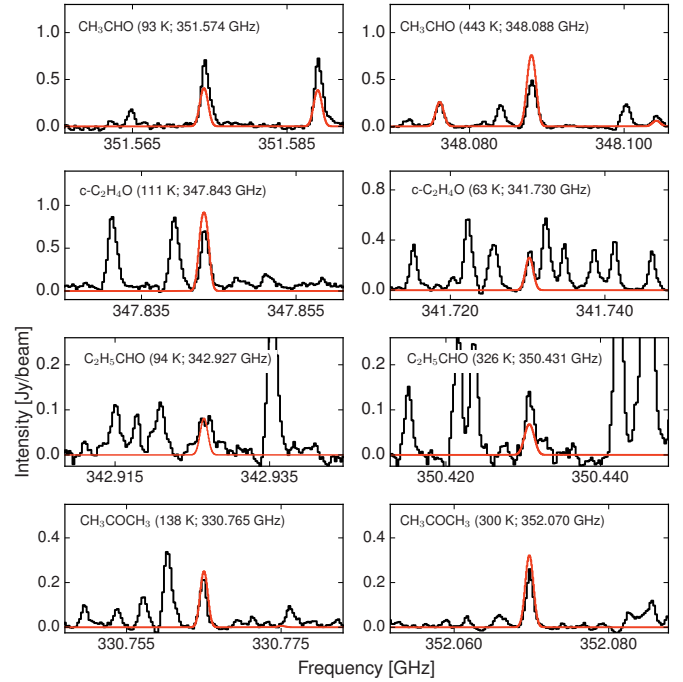


Fig. 2. Observed and synthetic spectra of the representative transitions shown in Fig. 1. The observed spectra are extracted at a position ($-0.45''$; $-0.30''$) southwest of the continuum peak of IRAS 16293B.

since the continuum is optically thick and very bright there are also very prominent absorption lines in the spectrum. To reduce the influence of absorption while still retaining as much intensity in the emission lines as possible, we extracted a spectrum from a position at $\alpha_{\text{J2000}} = 16^{\text{h}}32^{\text{m}}22.58^{\text{s}}$; $\delta_{\text{J2000}} = -24^{\circ}28'32''.8$, corresponding to an offset of ($-0.45''$; $-0.30''$) in the southwestern direction relative to the continuum peak of IRAS 16293B. This spectrum, corrected for the LSR velocity ($V_{\text{LSR}} = 2.7 \text{ km s}^{-1}$), is used throughout this paper. Figure 2 shows the observed spectra for each of the transitions from Fig. 1.

The heavy blending of emission lines at the sensitivity of ALMA complicates the identification and analysis of individual molecular species. For this purpose we therefore calculate synthetic spectra for our target molecules and their physical parameters are derived by fitting synthetic spectra to the data. For the purpose of excluding blended lines from the analysis, we create a reference model containing the synthetic spectrum of emission lines of previously detected complex organic molecules that are expected to be present in the warm gas toward the two sources (Bisschop et al. 2008; Jørgensen et al. 2011, 2012, 2016; Coutens et al. 2016). Superimposing the reference model spectrum onto the observed spectrum reveals if a line of interest is blended with any of these species. For our analysis we exclude lines that are severely blended, that is, where the peaks of the emission lines overlap. In addition, we have also checked the lines of interest against other species in the CDMS¹ and JPL² databases (Müller et al. 2001, 2005; Pickett et al. 1998) with the CASSIS³ software and do not find any clear overlap with any other potential interstellar species.

The synthetic spectra are computed following the approach described in Goldsmith & Langer (1999). We assume that the

¹ <http://www.astro.uni-koeln.de/cdms>

² <http://spec.jpl.nasa.gov/>

³ <http://cassis.irap.omp.eu/>

molecular excitation obeys local thermodynamic equilibrium (LTE), which is reasonable at the densities and scales of the ALMA observations toward IRAS 16293B (Jørgensen et al. 2016), and calculate a synthetic spectrum of all transitions from a molecule given a line width, column density, rotational temperature, and source size, assuming Gaussian line profiles. The spectroscopic data for propanal (Butcher & Wilson Jr. 1964; Hardy et al. 1982; Demaison et al. 1987) and ethylene oxide (Cunningham Jr. et al. 1951; Creswell & Schwendemann 1974; Hirose 1974; Pan et al. 1998; Medcraft et al. 2012) are available from the CDMS database, while the spectroscopic data for acetone (Groner et al. 2002) and acetaldehyde (Kleiner et al. 1996) are available from the JPL database.

For the analysis we started by identifying the brightest potential lines of each of the relevant species adopting a full width half maximum (FWHM) line width and the source size remained fixed at 1.0 km s^{-1} and $0.5''$, respectively. We then generated a synthetic spectrum by adjusting the temperature and column density (N_{tot}) until a good fit for those lines was obtained. From this a priori spectrum, we identified approximately ten reasonably non-blended and optically thin ($\tau \leq 0.1$) lines for each species, which we use to minimize the reduced chi-squared statistic:

$$\chi_{\text{red.}}^2 = \frac{1}{N} \sum_{i=1}^N \left(\frac{I_{\text{obs},i} - I_{\text{syn},i}}{\sigma_i} \right)^2, \quad (1)$$

where I_{obs} and I_{syn} are the intensities of the observed and synthetic emission lines, respectively, N is the number of lines analyzed and σ the RMS error. In the analysis, we varied the column density from $1.0 \times 10^{14} \text{ cm}^{-2}$ – $1.0 \times 10^{18} \text{ cm}^{-2}$ with small increments and the temperature from 100 K–400 K with increments of 25 K, generating a new synthetic spectrum at each increment to evaluate against the observed spectrum at the locations of the chosen lines. Since the emission lines are blended, the reduced χ^2 is only calculated for the average value of the channels at the very peak of the lines (corresponding to the predicted frequency of the peak $\pm 0.25 \text{ MHz}$), instead of over the entire Gaussian bell curve.

From the reduced χ^2 analysis, acetaldehyde and ethylene oxide show the best fit at $T_{\text{ex}} \approx 125 \text{ K}$, while it is difficult to constrain the excitation temperature for propanal and acetone. Our analysis shows that the column densities do not vary greatly with temperature for all species, except for acetone, where a $T_{\text{ex}} = 400 \text{ K}$ results in a column density a factor of ten higher than for $T_{\text{ex}} = 100 \text{ K}$. A comparison between the synthetic and observed spectrum for acetone reveals that an excitation temperature of approximately 200 K could still be in agreement with the observations, but that a T_{ex} of 300 K overproduces some of the lines. Since it appears that the molecules are spatially coexisting and trace the same gas, we therefore assume $T_{\text{ex}} = 125 \text{ K}$ for all molecules. The resulting column densities are summarized in Table 1 and the relative abundance ratios of the different isomers are listed in Table 2. The uncertainties of T_{ex} and N_{tot} are dominated by the assumptions that go into the analysis, that is, LTE and Gaussian line profiles, instead of the statistical error. Therefore, the uncertainties are estimated to $\sim 50\%$ and 25 K on the column density and the emission temperature, respectively.

Figures A.1–A.3 show the synthetic spectra of ethylene oxide, propanal, and acetone, respectively, as well as the reference model superimposed on the observed spectrum for all lines where the synthetic spectrum predicts a peak line intensity equal to or above twice the RMS noise of the spectrum. The lines are

Table 1. Best fit column densities.

Molecule		$N_{\text{tot}} [\text{cm}^{-2}]$
Acetone	CH_3COCH_3	1.7×10^{16}
Propanal	$\text{C}_2\text{H}_5\text{CHO}$	2.2×10^{15}
Acetaldehyde	CH_3CHO	7.0×10^{16}
Ethylene oxide	$\text{c-C}_2\text{H}_4\text{O}$	6.1×10^{15}

Notes. The results are derived assuming $\theta_{\text{source}} = 0.5''$, $T_{\text{ex}} = 125 \text{ K}$ and $\text{FWHM} = 1.0 \text{ km s}^{-1}$. The column density of propanal was corrected by a factor of 1.489 to take into account the vibrational and conformational contribution at $T = 125 \text{ K}$.

sorted into descending intensity. We check each line in the synthetic spectra against the observed spectrum for each molecule, and the majority of them provide a reasonable match, within the estimated uncertainty. We claim a detection for lines i) that are reasonably well separated from other species in the reference model and ii) where the integrated line strength over FWHM is larger than three times the statistical uncertainty ($\sqrt{n_{\text{chan}}} \times \text{RMS}$) of the line and iii) where there is a reasonably good fit between the synthetic and the observed spectrum. Table B.1 lists the spectroscopic catalog values, the integrated intensity over the FWHM for the observed spectrum, and the detection level for the detected lines of ethylene oxide, propanal, and acetone. The transitions are listed with increasing frequency and it should be noted that many of the detected lines are a blend of several internal rotation components.

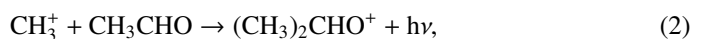
For ethylene oxide, propanal, and acetone, we detected 20, 44, and 186 lines, respectively. Some of the acetone lines predicted by the models appear to be either slightly shifted or missing. In some cases, this can be explained by the presence of absorption at the same frequency as the predicted lines, but in most cases these lines correspond to transitions with both high K_a and low K_c quantum numbers (see Table C.1). None of the missing or shifted lines with high K_a and low K_c numbers were used for the determination of the spectroscopic parameters. It was admitted by Groner et al. (2002) that these lines do not fit very well. It could be due to perturbations from interactions between the (high K_a , low K_c) levels and the levels from the lowest torsional excited states (Groner et al. 2002).

We also search for vinyl alcohol (Saito 1976), another isomer of acetaldehyde and ethylene oxide, but no detection can be claimed so far. With a conservative upper limit of $2 \times 10^{15} \text{ cm}^{-2}$ for the syn form (the lowest energy form of vinyl alcohol), this isomer is less abundant than acetaldehyde and ethylene oxide, similarly to what was found in Sgr B2 by Belloche et al. (2013).

4. Discussion

As described in the introduction, the relative abundances of the different isomers are important constraints on chemical models and provide insight into the formation of the complex species. Table 2 lists the different abundance ratios and Fig. 3 gives a schematic overview of the entries from the table. A number of different formation pathways have been proposed for the studied species.

For acetone, the ion-molecule radiative association reaction



followed by



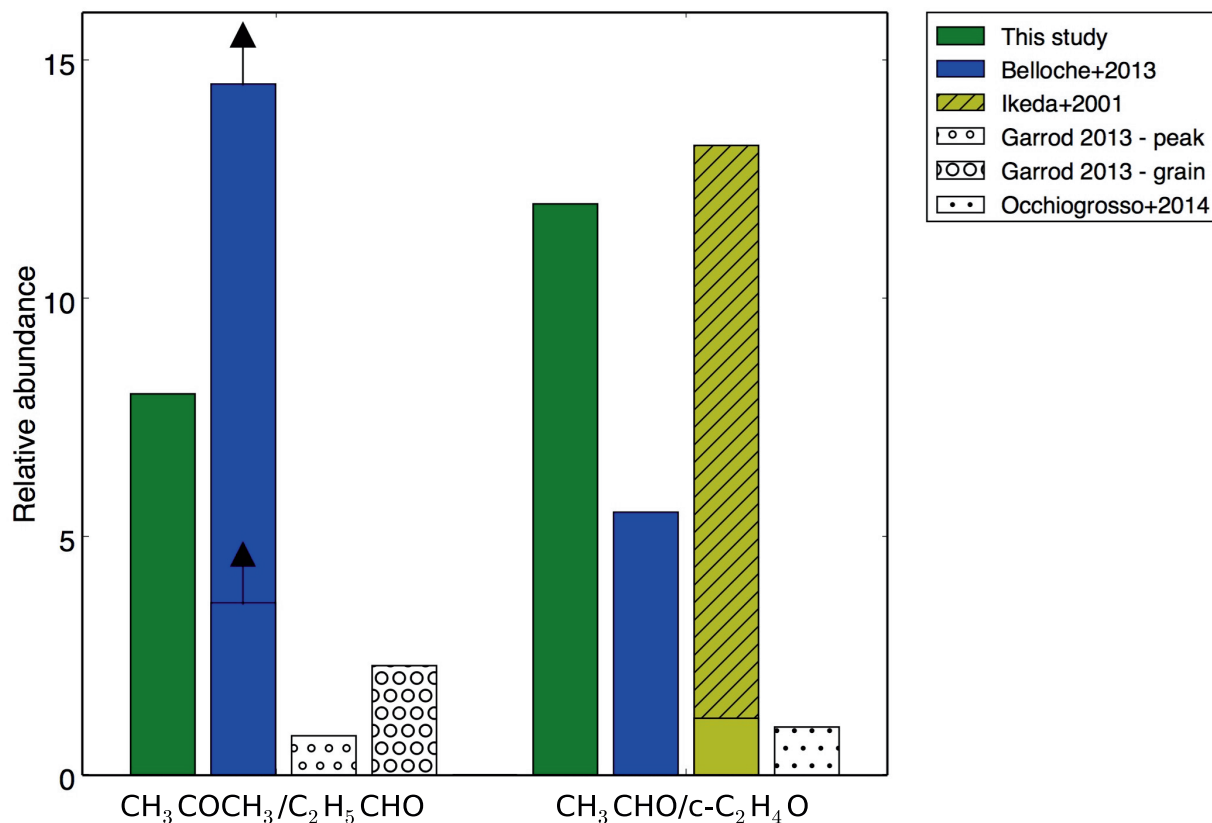


Fig. 3. Bar plot of the relative abundances of $\text{CH}_3\text{COCH}_3/\text{C}_2\text{H}_5\text{CHO}$ and $\text{CH}_3\text{CHO}/\text{c-C}_2\text{H}_4\text{O}$ from Table 1. The observations are indicated by color bars, while the chemical predictions are shown by white bars with different circle sizes. The two lower limits derived by Belloche et al. (2013) for $\text{CH}_3\text{COCH}_3/\text{C}_2\text{H}_5\text{CHO}$ are illustrated by upward arrows. The range of $\text{CH}_3\text{CHO}/\text{c-C}_2\text{H}_4\text{O}$ ratios determined in ten sources by Ikeda et al. (2001) is indicated by the hatched area. For the $\text{CH}_3\text{CHO}/\text{c-C}_2\text{H}_4\text{O}$ ratio from Belloche et al. (2013), we used the average value of the column densities of the rotational and first torsionally ($\nu_t = 1$) excited states of acetaldehyde.

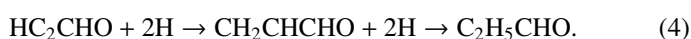
Table 2. Relative abundances in different sources.

Source	$\text{CH}_3\text{COCH}_3/\text{C}_2\text{H}_5\text{CHO}$	$\text{CH}_3\text{CHO}/\text{c-C}_2\text{H}_4\text{O}$	References
IRAS 16293-2422	8	12	this study
Sgr B2(N)	$\geq 3.6\text{--}14.5^a$	$3.7\text{--}7.4^b$	Belloche et al. (2013)
Survey of massive SF regions	–	$1.2\text{--}13.2$	Ikeda et al. (2001)
Chemical model: peak gas-phase	$0.22: 0.83: 0.07^c$	–	Garrod (2013)
Chemical model: peak grain-surface	$0.37: 2.3: 0.39^c$	–	Garrod (2013)
Chemical model of hot cores	–	1^d	Occhiogrosso et al. (2014)

Notes. ^(a) Range reflects span for rotational states in the $V_{\text{off}} = 0 \text{ km s}^{-1}$ and the $V_{\text{off}} = 10 \text{ km s}^{-1}$ components of Sgr B2(N). Propanal is not detected, therefore the upper limit is used after correction for a similar beam filling factor. ^(b) Range reflects span for the rotational and first torsionally ($\nu_t = 1$) excited states of acetaldehyde in the $V_{\text{off}} = -1 \text{ km s}^{-1}$ component of Sgr B2(N). ^(c) Chemical model of hot cores for a slow, medium, and fast model, respectively. ^(d) The MONACO code (at 200 K and $1.2 \times 10^6 \text{ yr}$).

proposed by Combes et al. (1987) has been shown not to be efficient enough to produce the observed values (Herbst et al. 1990). In the model presented by Garrod et al. (2008), acetone is formed on grains by the addition of CH_3 to CH_3CO .

Hollis et al. (2004) proposed the formation of propanal to occur through simple successive hydrogenation:



However, Garrod (2013) proposed a different formation route through the addition of HCO and C_2H_5 radicals on grains. Garrod (2013) found the formation to be most rapid at 30 K,

when sublimation of grain-surface methane (CH_4) is most efficient.

Laboratory experiments were conducted by Bennett et al. (2005a,b) to study the synthesis of acetaldehyde, ethylene oxide, and vinyl alcohol in interstellar and cometary ices after irradiation with energetic electrons. Acetaldehyde appeared to be formed in both CO-CH_4 and $\text{CO}_2\text{-C}_2\text{H}_4$ ice mixtures, while ethylene oxide and vinyl alcohol are only detected in $\text{CO}_2\text{-C}_2\text{H}_4$ ice mixtures (Bennett et al. 2005a,b). While CO, CO_2 , and CH_4 have been observed in interstellar ices, C_2H_4 is formed as a secondary product by charged particle irradiation and photolysis of CH_4 ices and it is therefore likely only present in small

concentrations (Bennett et al. 2005b) although it may be formed through gas-phase mechanisms under cold, dense conditions. Thus, assuming the relative production rates of acetaldehyde, ethylene oxide and vinyl alcohol are similar, the fractional abundance of acetaldehyde is expected to be higher than that of ethylene oxide and vinyl alcohol (Bennett et al. 2005b).

4.1. Propanal and acetone

We have compared our results to predictions from the three-phase (mantle/surface/gas) astrochemical kinetics model, MAGICKAL (Model for Astrophysical Gas and Ice Chemical Kinetics And Layering), as presented in Garrod (2013). By applying a chemical network to hot-core conditions, the model follows the physico-chemical evolution of a parcel of material from the core from the free-fall collapse of the cloud to the subsequent warm-up phase of the dense core from 8 to 400 K (Garrod 2013). MAGICKAL employs a (modified) rate-equation approach to solve the coupled ice mantle, ice-surface, and gas-phase chemistry allowing radicals on the grains to meet via thermal diffusion at intermediate temperatures and form more complex molecules prior to the complete sublimation of the dust-grain ice at higher temperatures. Garrod (2013) uses three different warm-up models: *fast*, *medium* and *slow*. Here we compare our results to all three models, but note that the fast warm-up model should, in principle, be the best match to the observations because the time for this model to reach 200 K is 5×10^4 yr which is comparable to the dynamical age of $\sim 1\text{--}3 \times 10^4$ yr for IRAS 16293 as derived by Schöier et al. (2002).

Garrod (2013) finds relative peak gas-phase abundances of $\text{CH}_3\text{COCH}_3/\text{C}_2\text{H}_5\text{CHO}$ of 0.22, 0.83, and 0.07 for the fast, medium and slow model, respectively. All three models predict a higher abundance of propanal compared to acetone, which is the opposite trend of our ratio of eight. Also, the upper limit toward Sgr B2(N) reported by Belloche et al. (2013) translates into a lower limit for $\text{CH}_3\text{COCH}_3/\text{C}_2\text{H}_5\text{CHO}$ of 3.6, which is consistent with our findings. One explanation may be that the model of Garrod (2013) uses a relatively low binding energy for acetone (3500 K), producing a desorption temperature of approximately 70 K. As discussed by Garrod et al. (2008), this low-temperature desorption results in rapid destruction of acetone in the gas-phase. Our observational fit to the excitation temperature of 125 K suggests that acetone is more likely desorbed from grains at the higher temperatures more commonly associated with complex organics, which would allow the majority of grain-surface formed acetone to survive for a significant period in the gas phase.

If we compare the peak *grain-surface* abundances of acetone and propanal produced in the Garrod (2013) chemical model which would be more representative of this situation, ratios of 0.37, 2.3, and 0.39 are obtained, respectively. The quantities of acetone and propanal produced on grains in the model are, in the case of the intermediate warm-up timescale, only a factor of a few below the observed ratio. However, it should be borne in mind that the efficient production of acetone depends, in this model, on the rate at which the CH_3CO radical may be produced on the grains. This may be achieved either through direct photodissociation of CH_3CHO or by the abstraction of a H-atom from this molecule by OH or NH_2 . The rates of each of these processes are not well defined by experiment, and these uncertainties could easily induce a variation in acetone production of a few factors. It is also likely that the physical conditions, which in the Garrod (2013) model are generic, representative hot-core conditions, may not be accurate for the specific case of IRAS 16293.

4.2. Ethylene oxide and acetaldehyde

Ikeda et al. (2001) searched for acetaldehyde and ethylene oxide in several massive star-forming regions. They detect both molecules in ten sources and find $\text{CH}_3\text{CHO}/\text{c-C}_2\text{H}_4\text{O}$ spanning a range from 1.2 in Sgr B2(N) to 13.2 in W51e1/e2. Belloche et al. (2013) also observed these molecules towards Sgr B2(N) and found a slightly higher value than Ikeda et al. (2001) of 3.7–7.4. It thus seems that our observed value of 12 in a low-mass YSO is toward the high end of the range observed in these high-mass regions, but that source-to-source variations may be larger than between the different groups of sources.

Occhiogrosso et al. (2014) used a two-stage (grain/gas) model, MONACO, to predict the gaseous acetaldehyde and ethylene oxide abundances during the cooling-down and subsequent warm-up phase of a hot core. At 200 K and 1.2×10^6 yr, the fractional abundance of ethylene oxide and acetaldehyde with respect to total H is 2×10^{-9} for both molecules, which means that the relative abundance between the two species is unity. As previously mentioned, based on their laboratory experiments, Bennett et al. (2005a,b) expect the relative abundance of $\text{CH}_3\text{CHO}/\text{c-C}_2\text{H}_4\text{O}$ to be larger than unity. Again, it seems that there are some variations in the observed acetaldehyde-to-ethylene oxide ratios, and that the model results of Occhiogrosso et al. (2014) best reproduce the lower end in that range, while our measurements are at the opposite end, more than an order of magnitude above. Nevertheless, given the variations seen in the models for acetone and propanal, whether the specific physical structures of the sources can be part of the explanation remains to be explored.

5. Conclusion

We have carried out the first investigation of the oxygen bearing species in the ALMA PILS survey of the protostellar binary system IRAS 16293. Our main findings are summarized as follows:

1. We have detected the molecules ethylene oxide ($\text{c-C}_2\text{H}_4\text{O}$), acetone (CH_3COCH_3), and propanal ($\text{C}_2\text{H}_5\text{CHO}$) for the first time toward a solar-type protostar. We have verified that the emission of these species, along with acetaldehyde (CH_3CHO), originates from the compact central region of the protostar, which confirms our assumption that these molecules spatially coexist. We determined a common excitation temperature, $T_{\text{ex}} \approx 125$ K for all four molecules and use this to determine column densities for each species.
2. Compared to previous observations, our results for the relative abundance ratio of $\text{CH}_3\text{COCH}_3/\text{C}_2\text{H}_5\text{CHO}$ are consistent with the lower limit found by Belloche et al. (2013) of SgrB2(N). The ratio for $\text{CH}_3\text{CHO}/\text{c-C}_2\text{H}_4\text{O}$ is comparable to the largest value in the span of observed values of high-mass sources from Ikeda et al. (2001) (variation between the sources in that sample of approximately an order of magnitude). This suggests that the chemistry in the most central part of IRAS 16293 (the hot corino region) is not significantly different from those of the high-mass hot cores, but that there may still be measurable source-to-source variations.
3. Contrary to our result, the models in Garrod (2013) predict propanal to be more abundant than acetone, except for the peak grain-surface abundances in the medium warm-up model, where the prediction is only few factors different from our result. Occhiogrosso et al. (2014) find the ratio of $\text{CH}_3\text{CHO}/\text{c-C}_2\text{H}_4\text{O}$ to be unity which is consistent with the

lowest observed value of a high-mass star forming region (Ikeda et al. 2001). All of the models investigated here return low relative abundances compared to our results, but they are however in reasonable agreement with the lowest value in the ranges reported by Ikeda et al. (2001) and Belloche et al. (2013).

The results from this paper imply that although the chemical models can reproduce the observations for some high-mass protostars reasonably well, they need to be modified to reflect the observed range of values for high-mass sources as well as our low-mass source. As discussed, the models would improve with better-defined reaction rates while including more species in the chemical networks could also improve model predictions. More observations, in particular toward low-mass sources, are needed for comparison with models to further constrain the formation pathways.

The detections also demonstrate the great potential of spectral surveys such as PILS for identifying new species that have so far gone undetected toward solar-type stars. New detections of complex organic molecules and the determination of their relative abundances for the first time in a solar-type protostar is important because it substantiates the chemical complexity of IRAS 16293 and can be used to constrain astrochemical models. The relative abundances reveal information of the formation pathway of the molecules and enable comparisons with models and laboratory experiments. In addition, the comparison of the ratios found in high-mass sources and low-mass protostars is vital to understanding the environmental effects on the formation of different molecular species.

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Appendix A: Observed and synthetic spectra

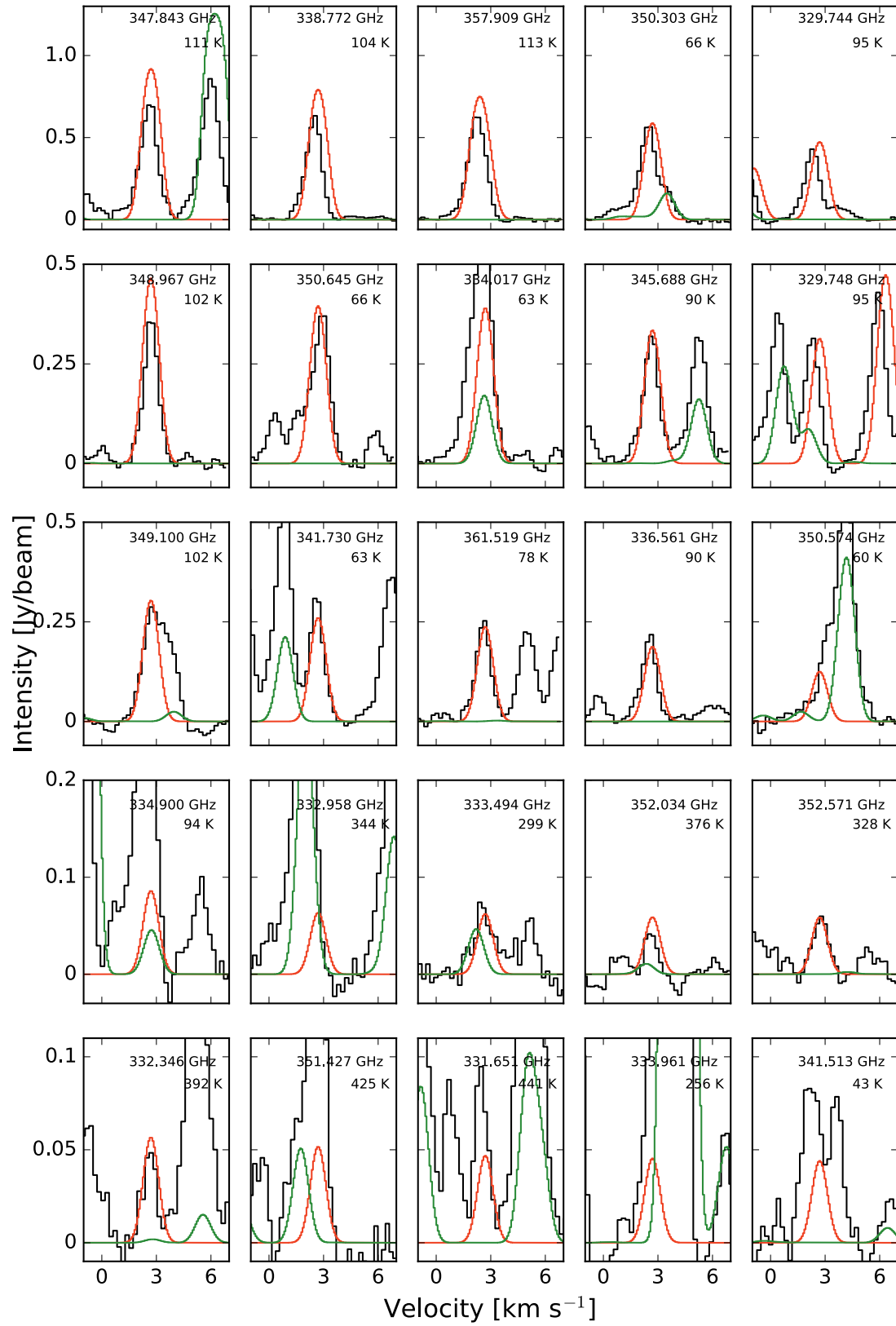


Fig. A.1. Ethylene oxide (c-C₂H₄O): synthetic spectrum in red and reference model in green superimposed onto observed spectrum.

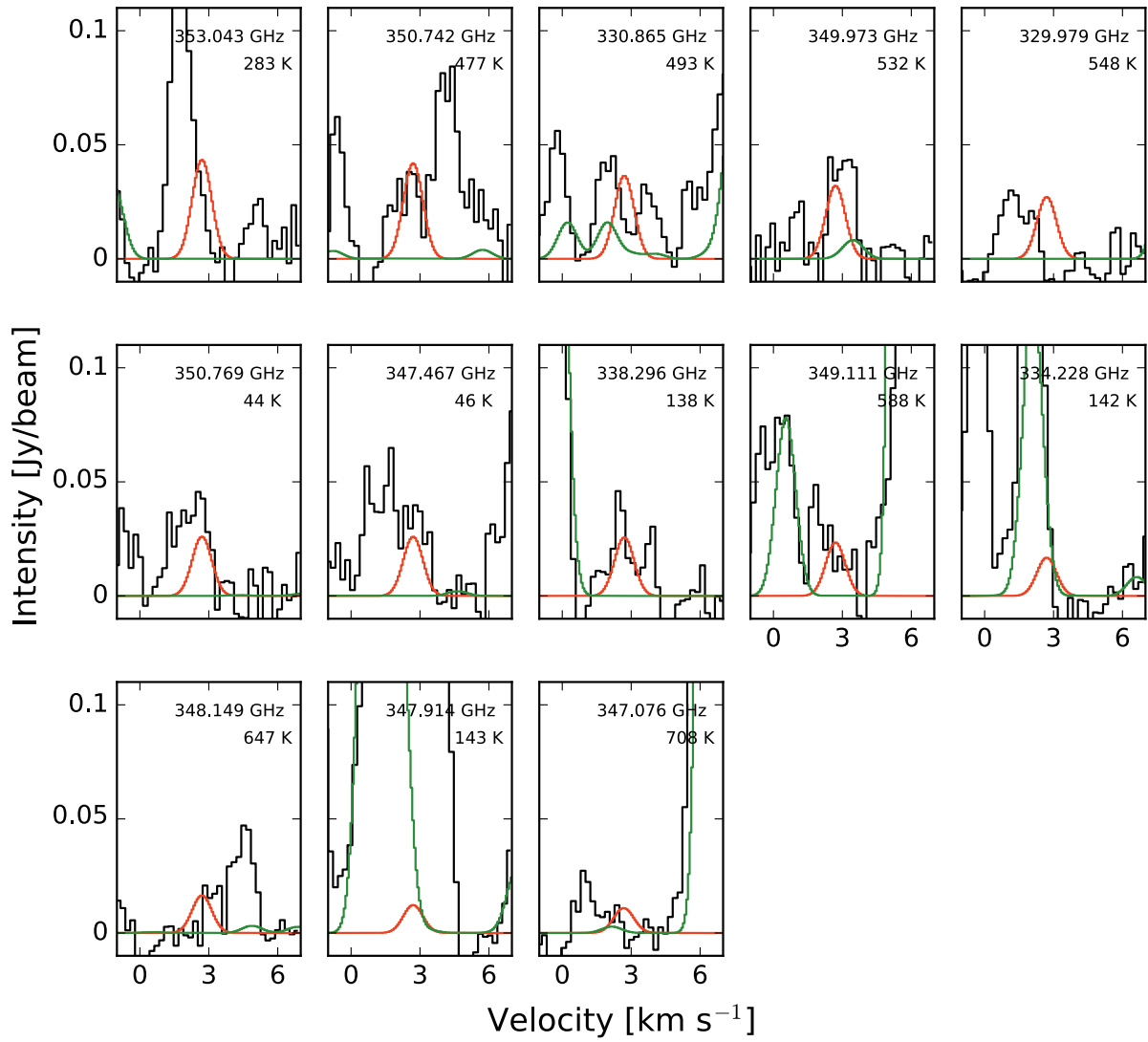


Fig. A.1. continued.

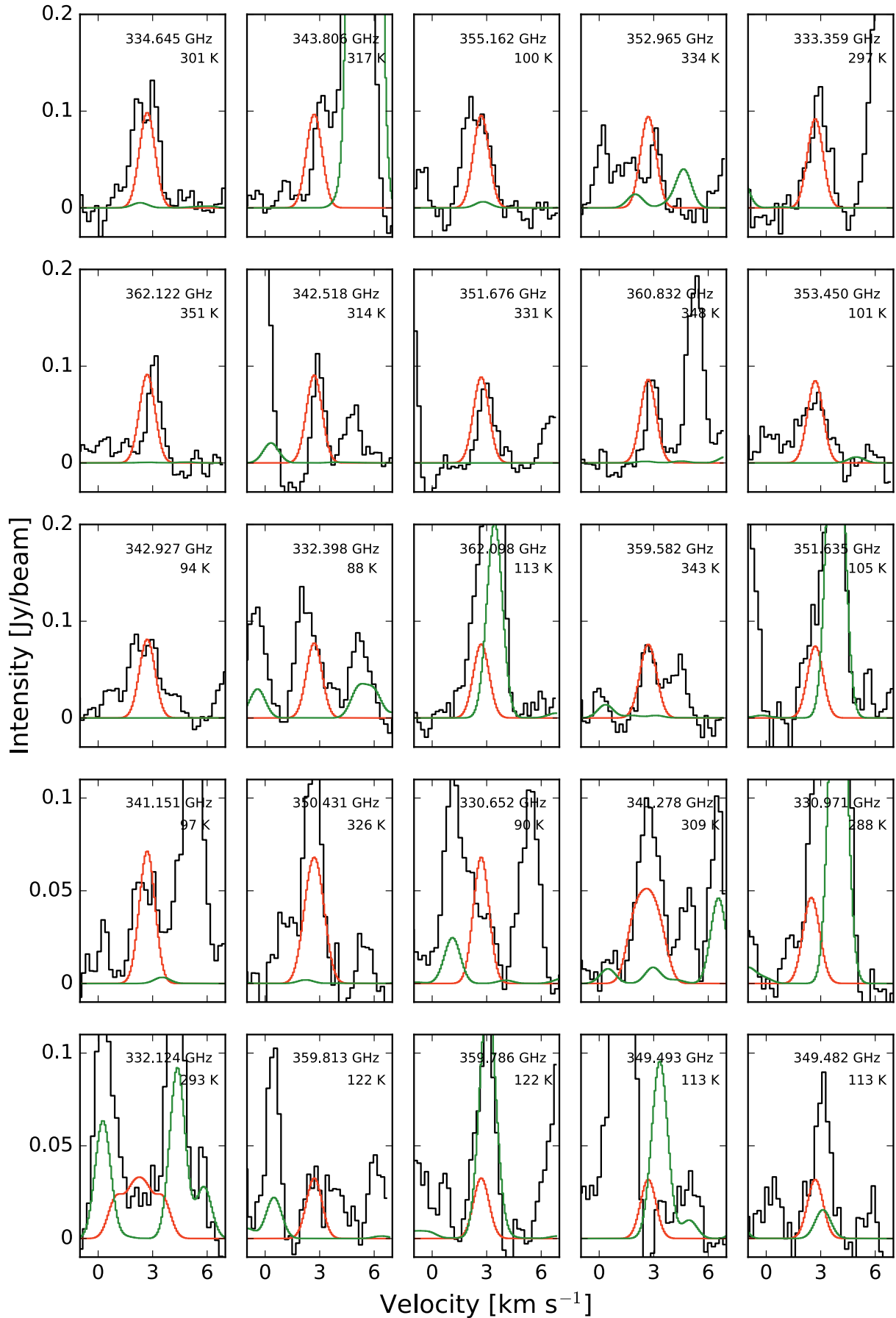


Fig. A.2. Propanal ($\text{C}_2\text{H}_5\text{CHO}$): synthetic spectrum in red and reference model in green superimposed onto observed spectrum.

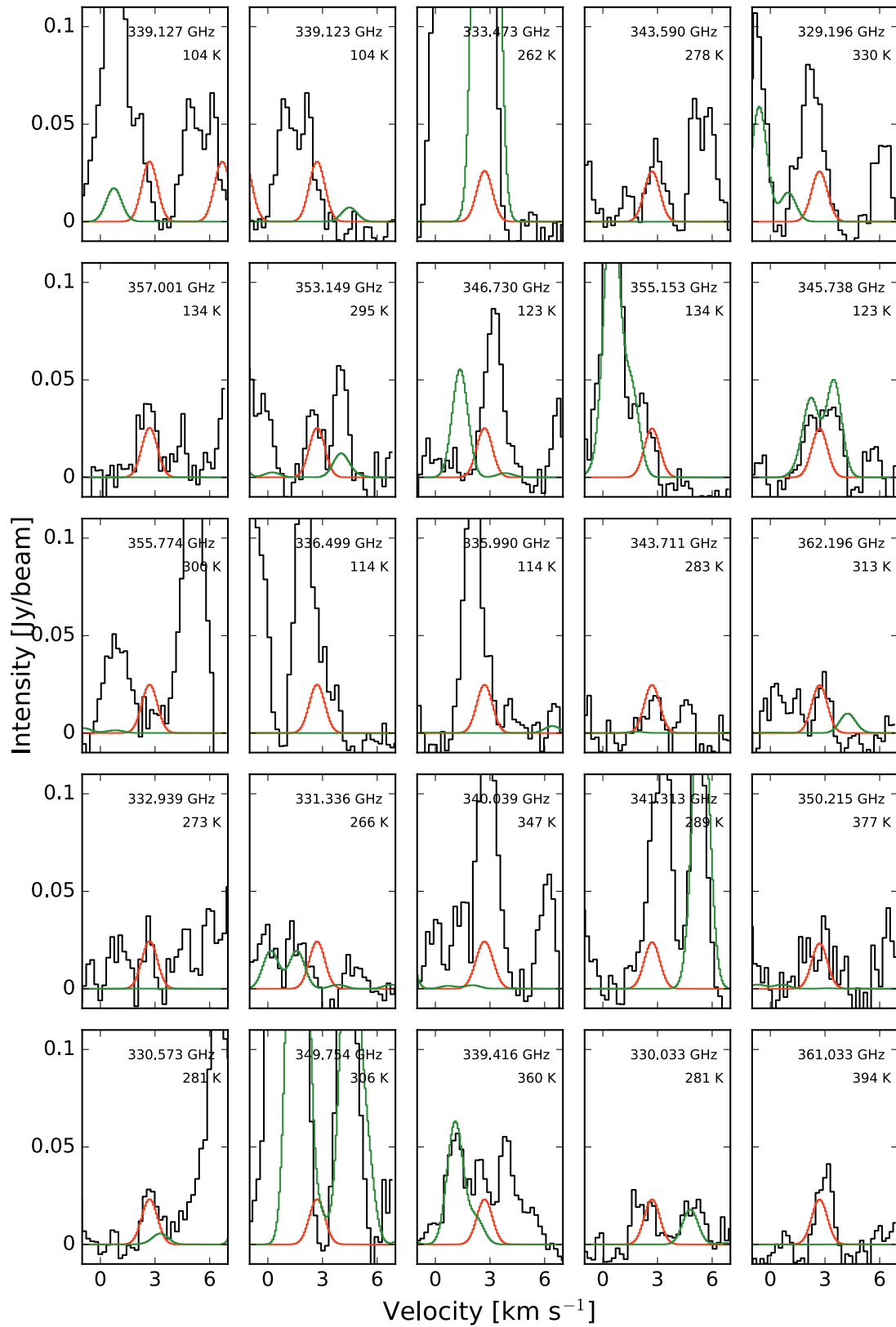


Fig. A.2. continued.

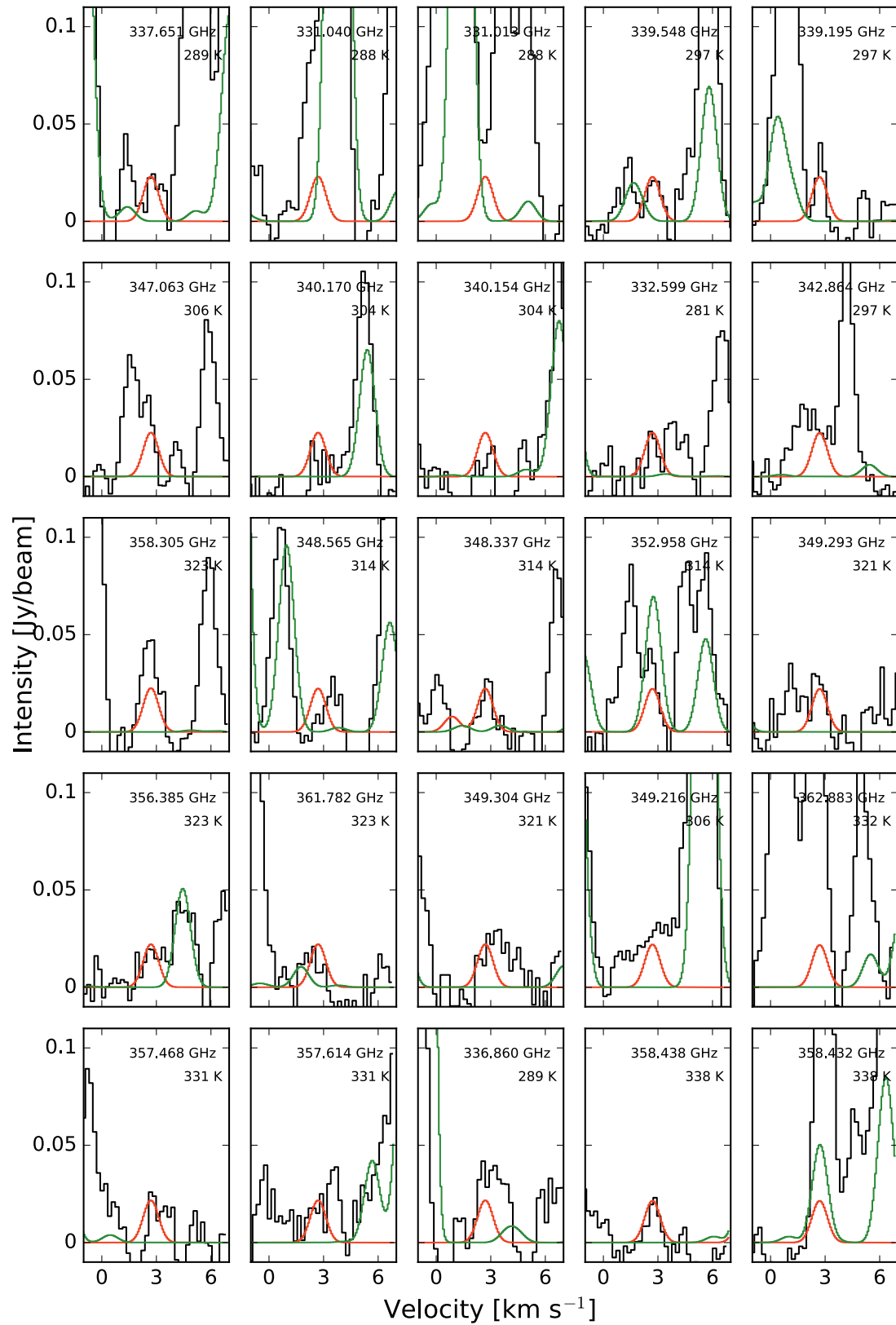


Fig. A.2. continued.

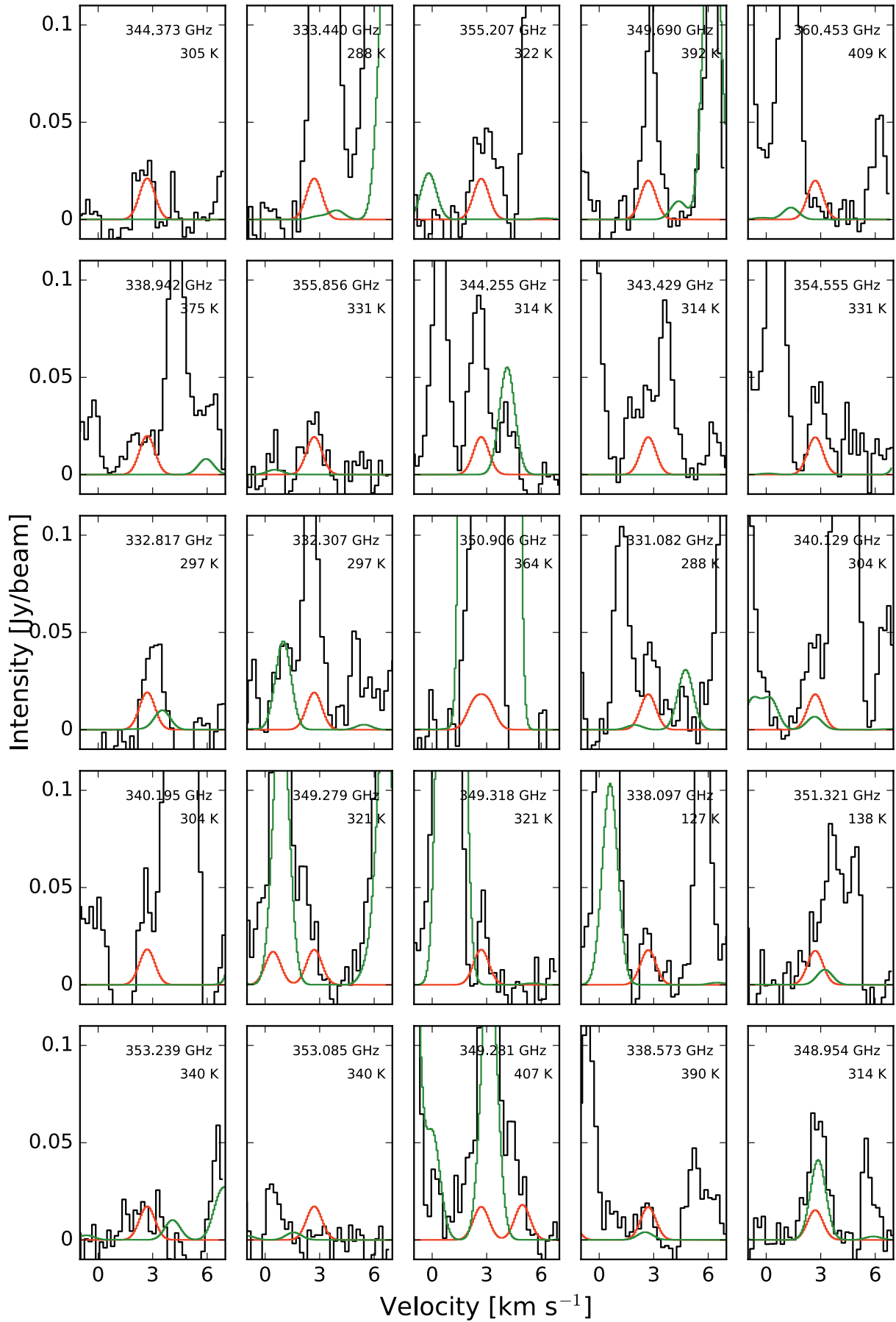


Fig. A.2. continued.

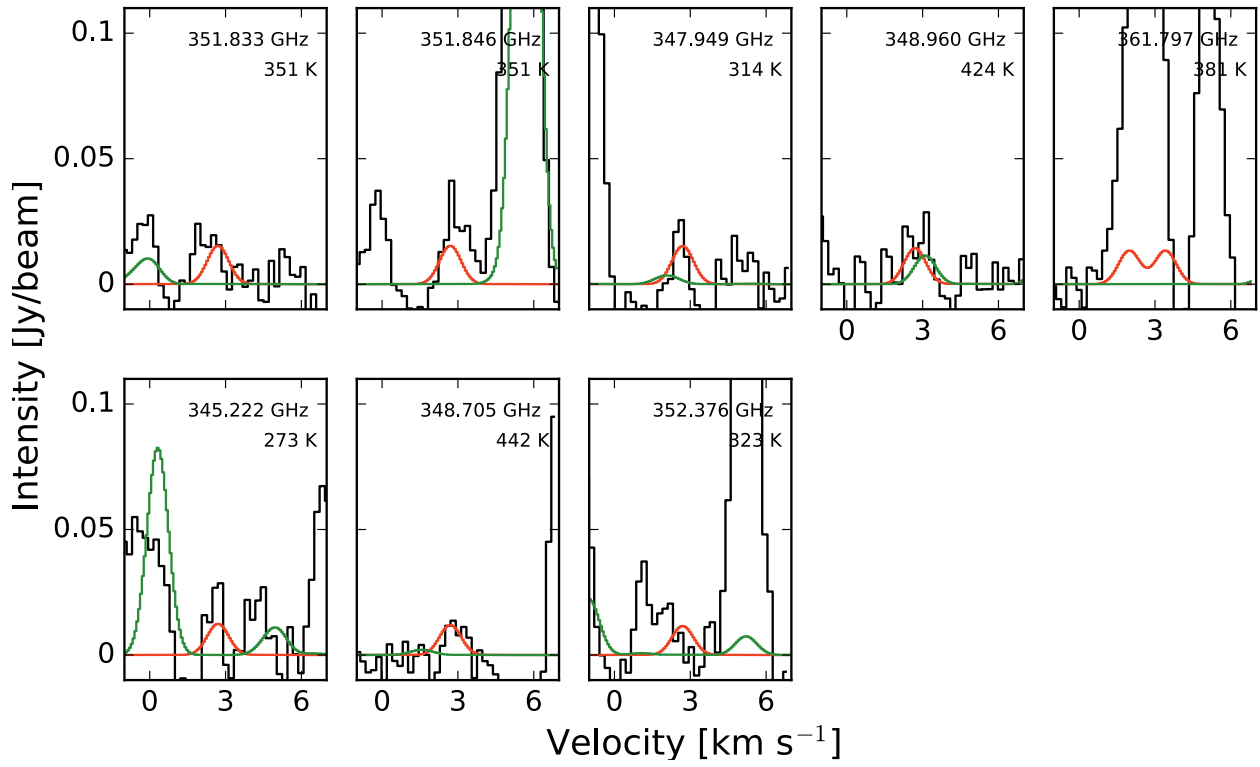


Fig. A.2. continued.

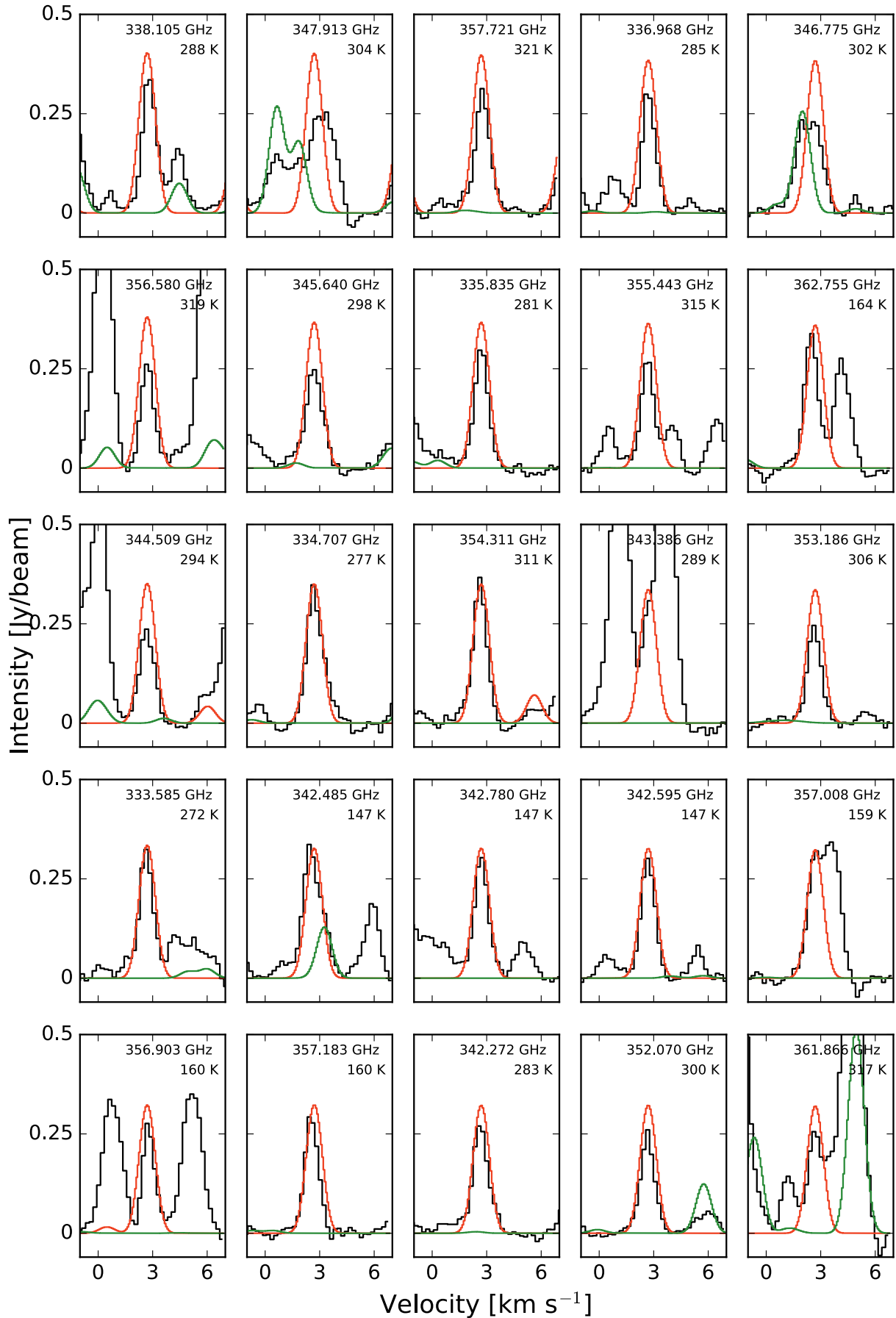


Fig. A.3. Acetone (CH_3COCH_3): synthetic spectrum in red and reference model in green superimposed onto observed spectrum.

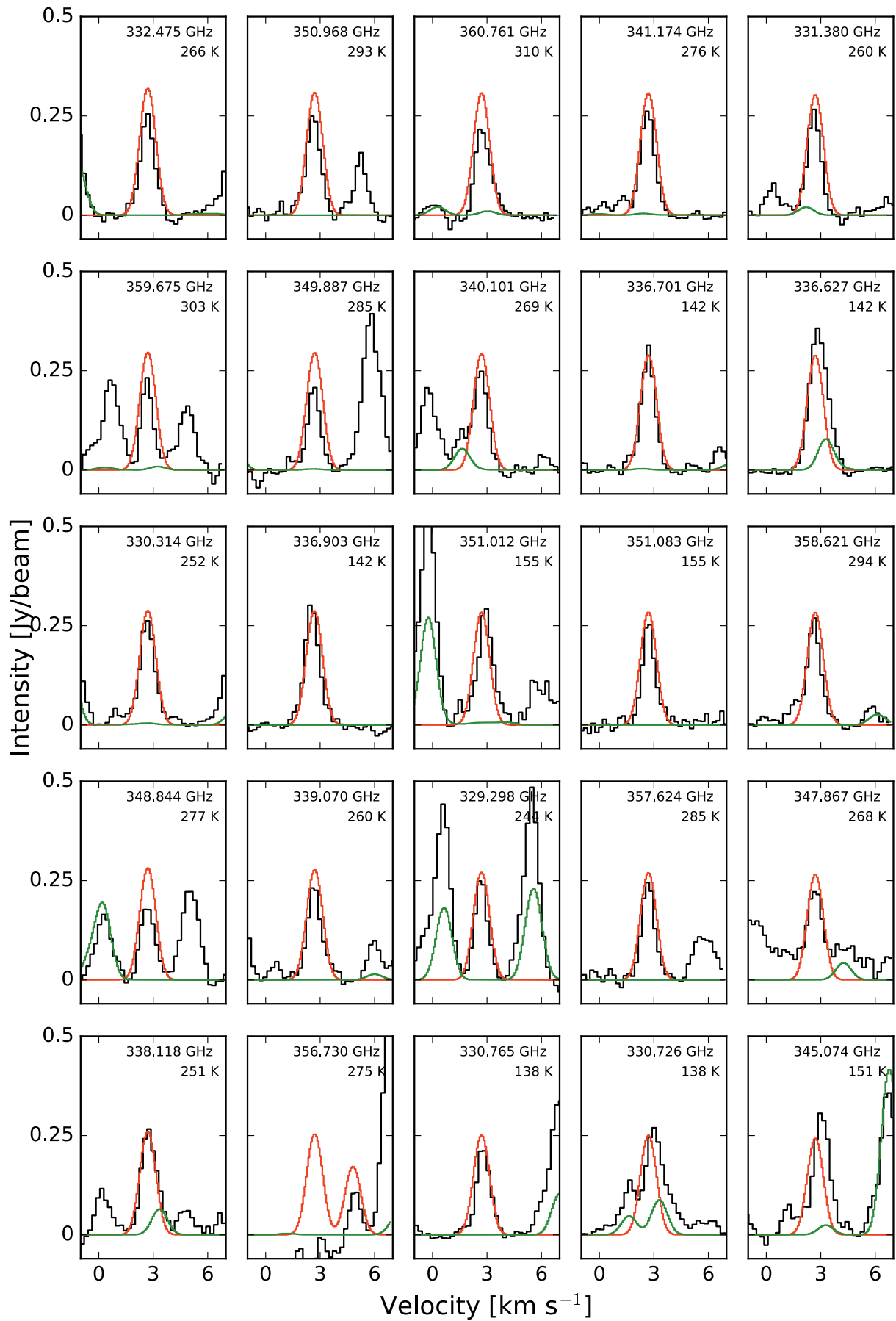


Fig. A.3. continued.

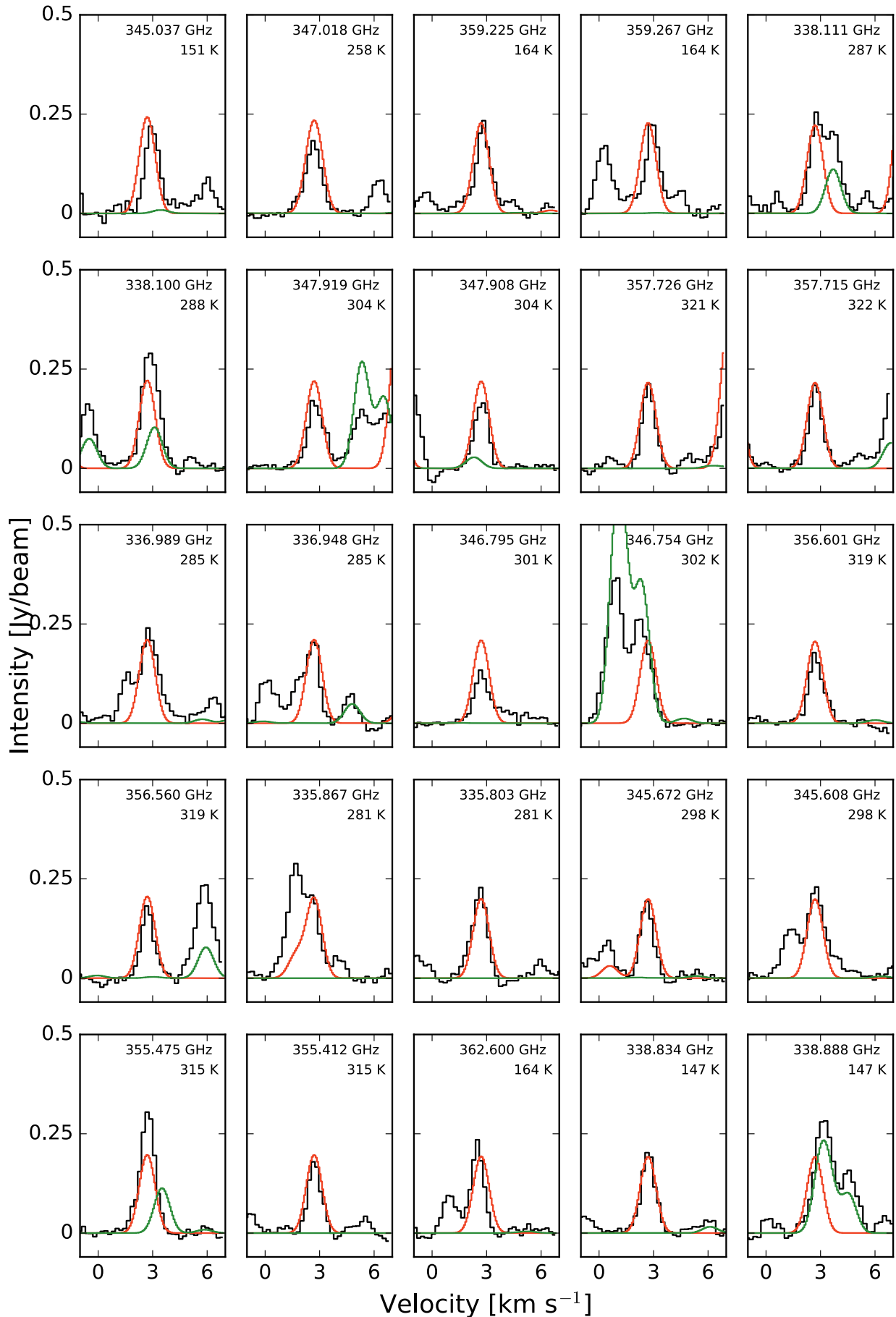


Fig. A.3. continued.

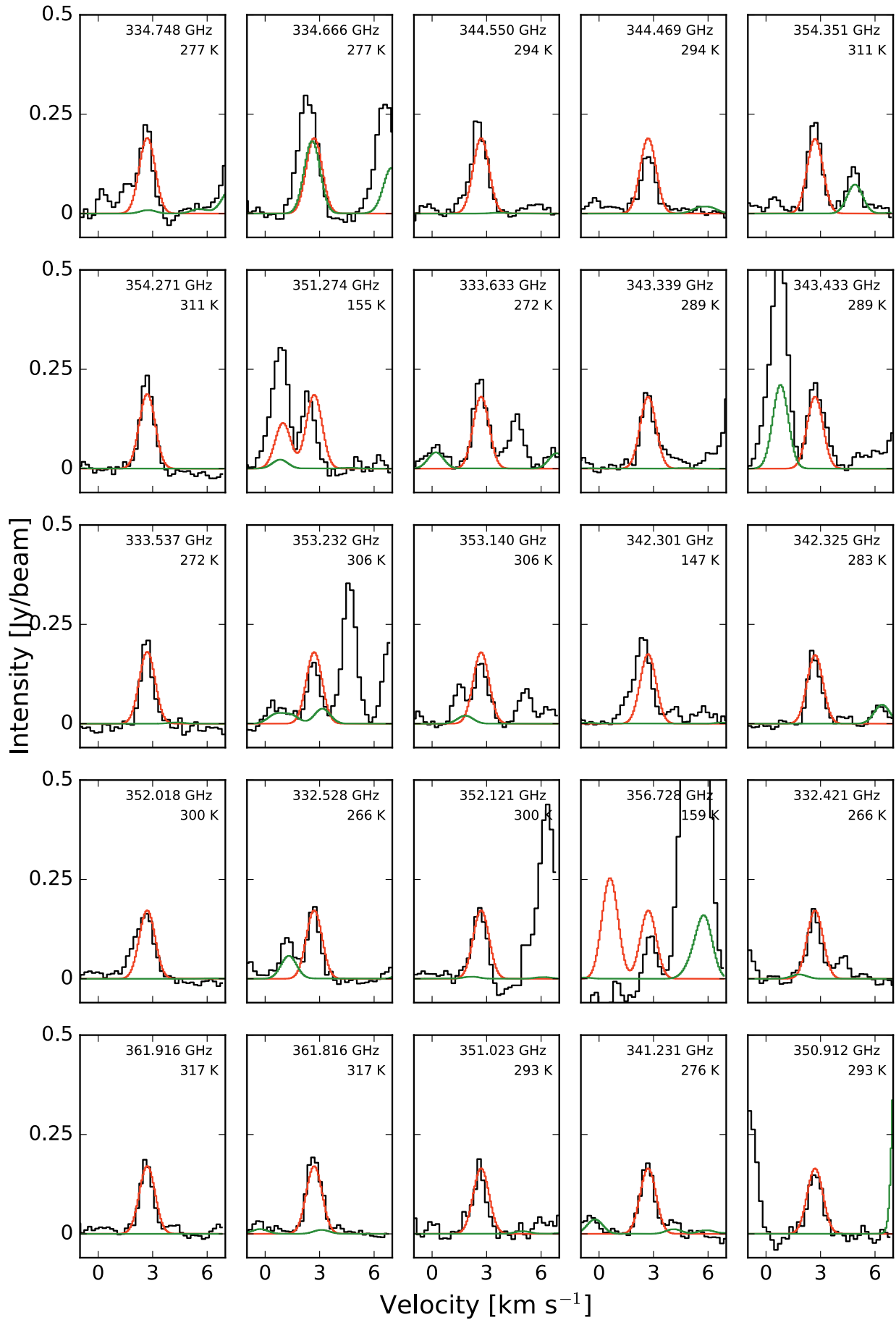


Fig. A.3. continued.

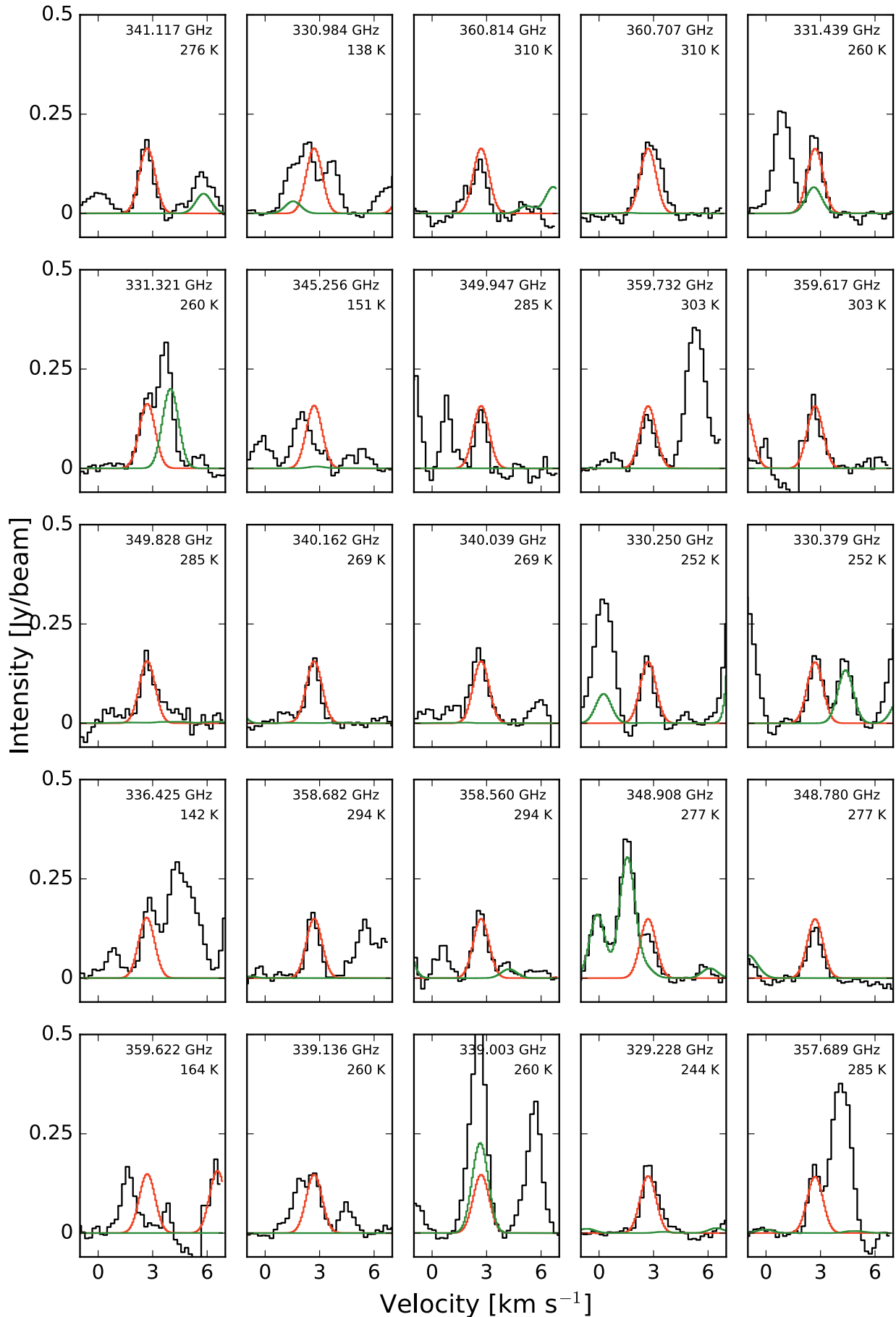


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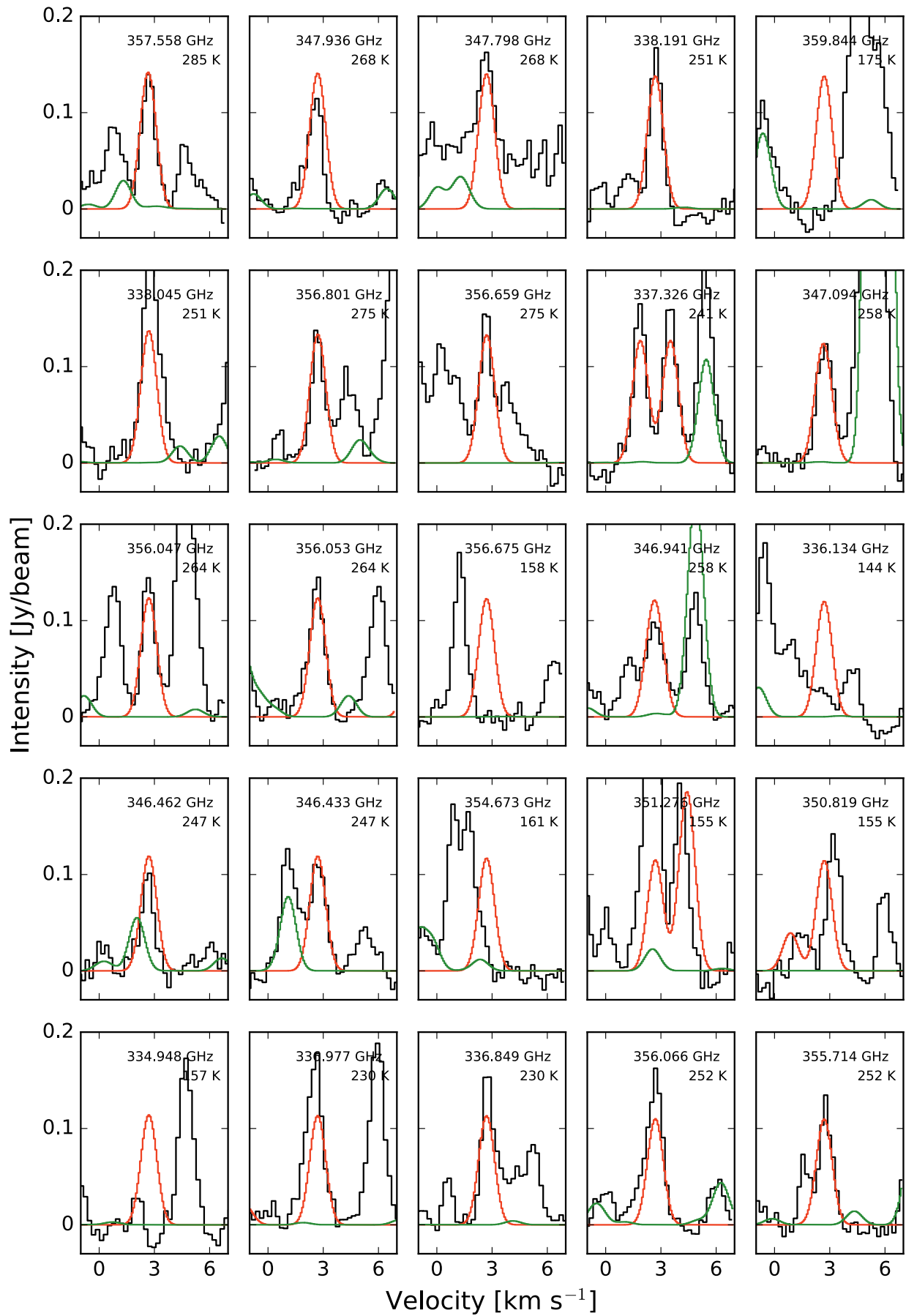


Fig. A.3. continued.

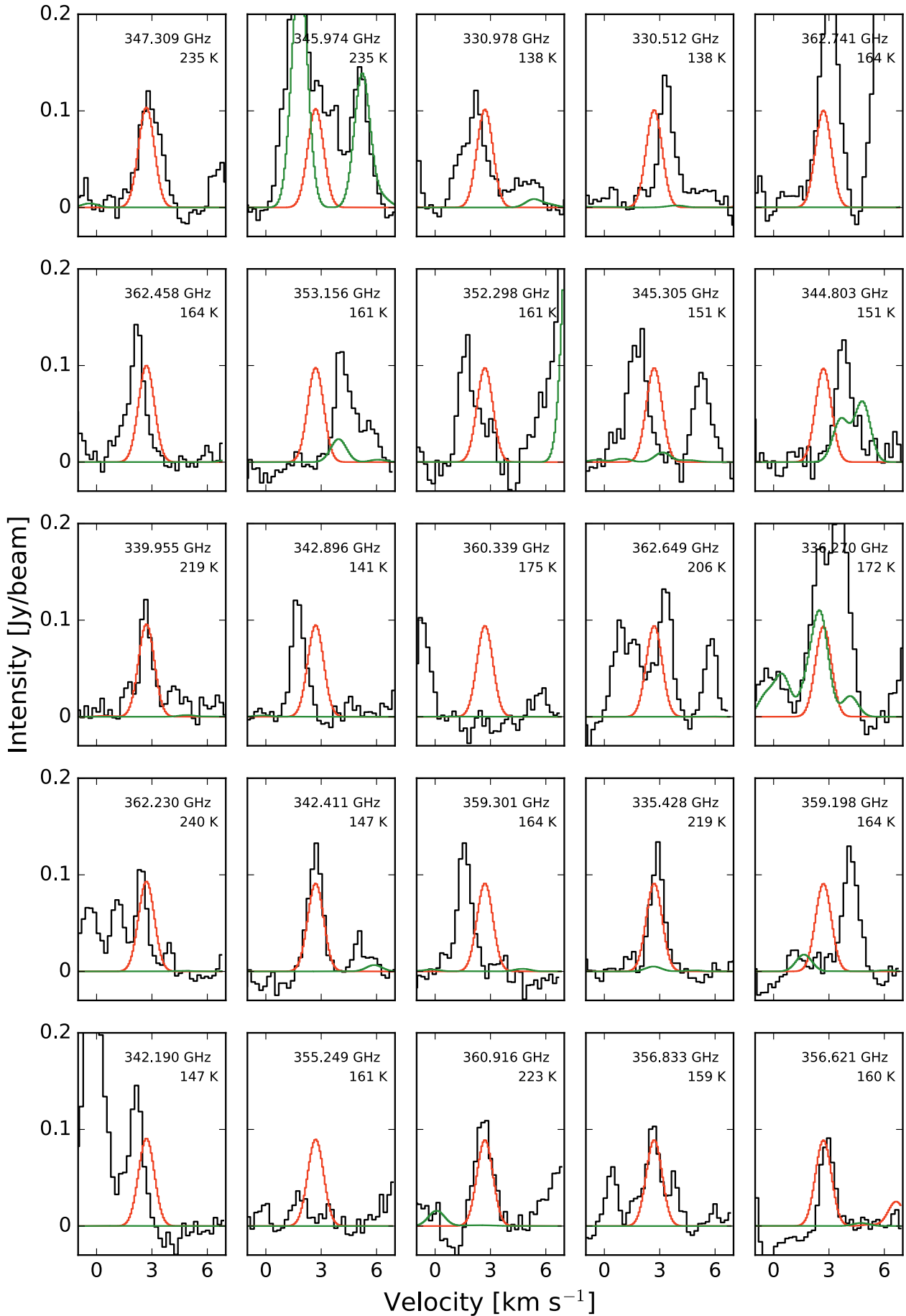


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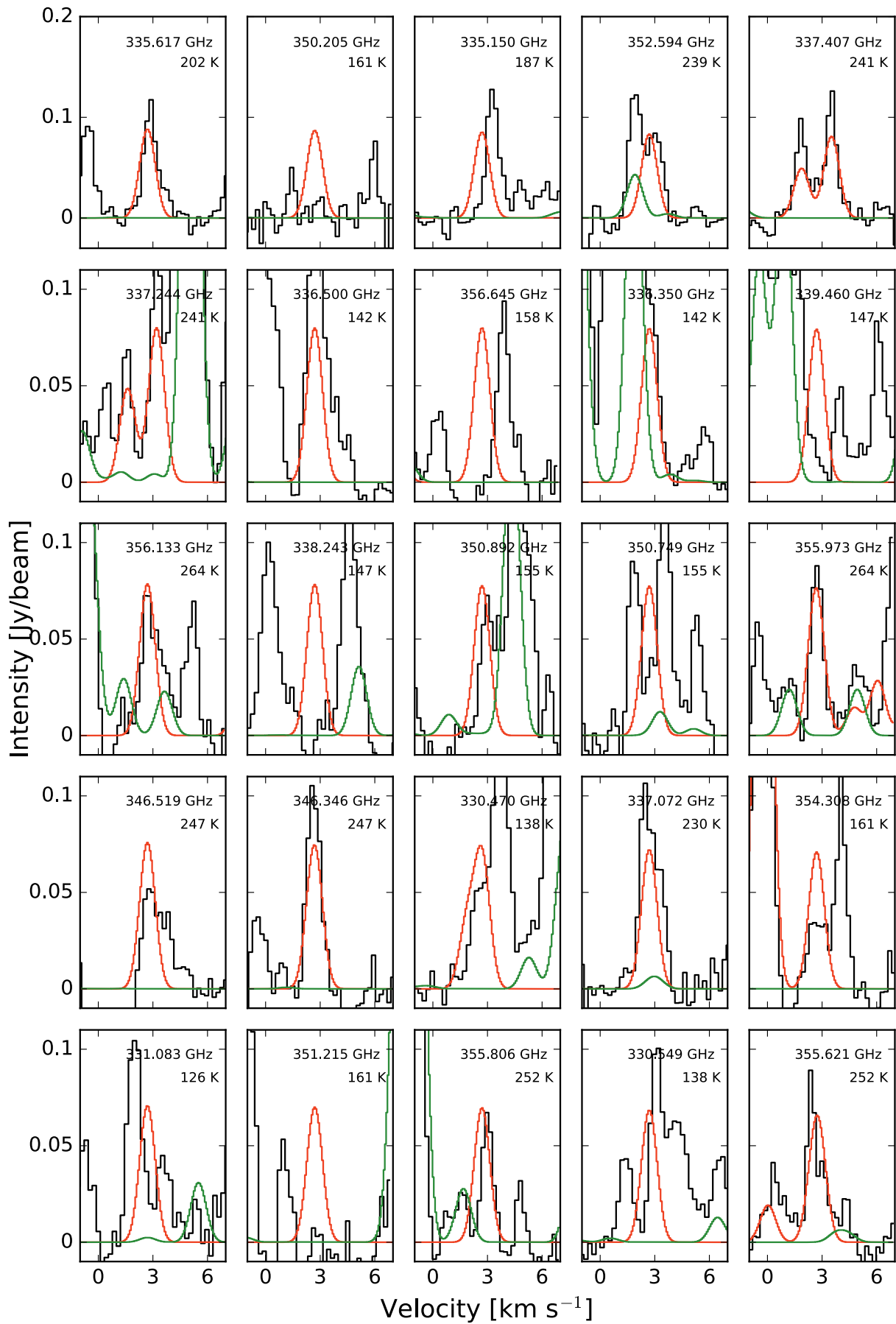


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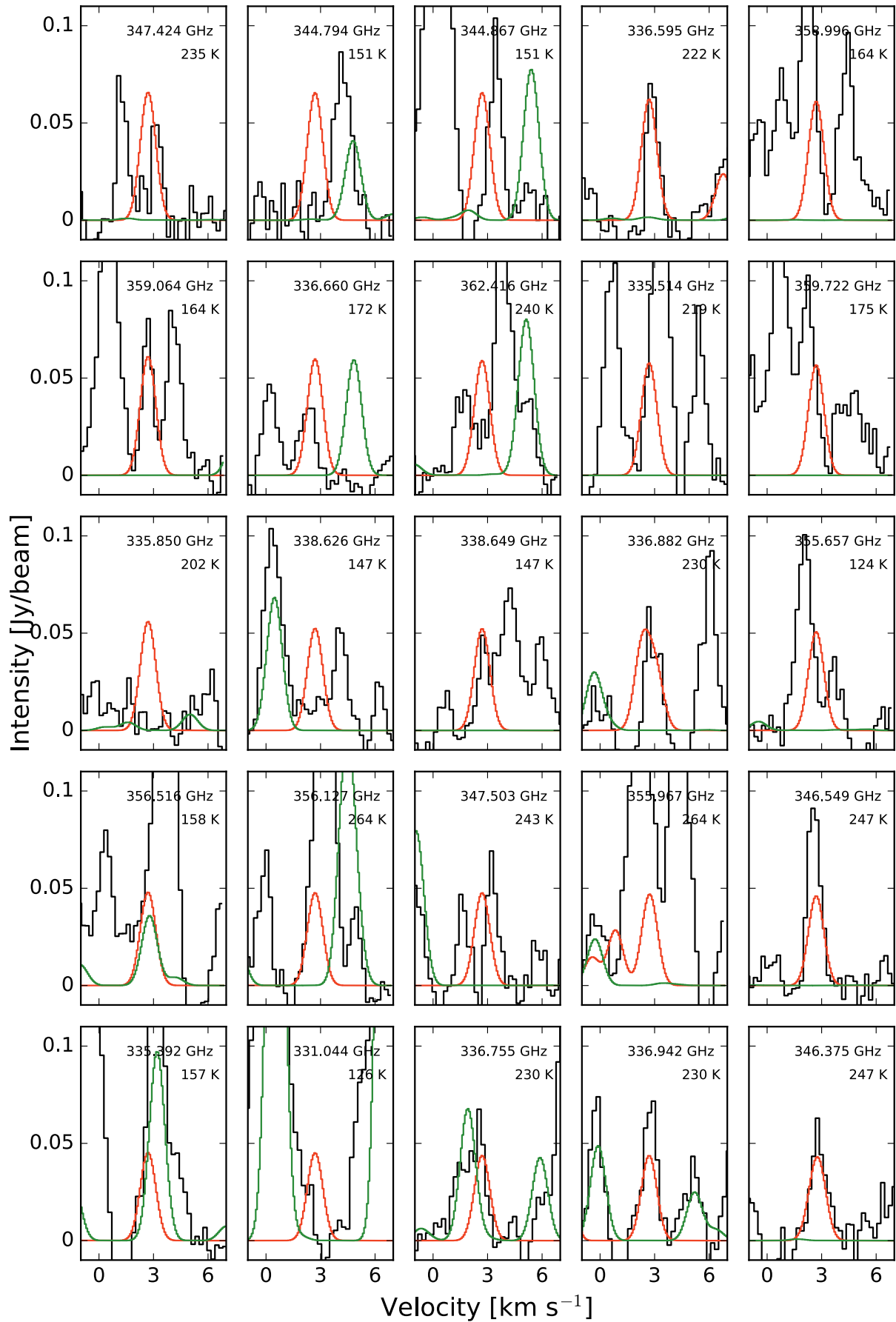


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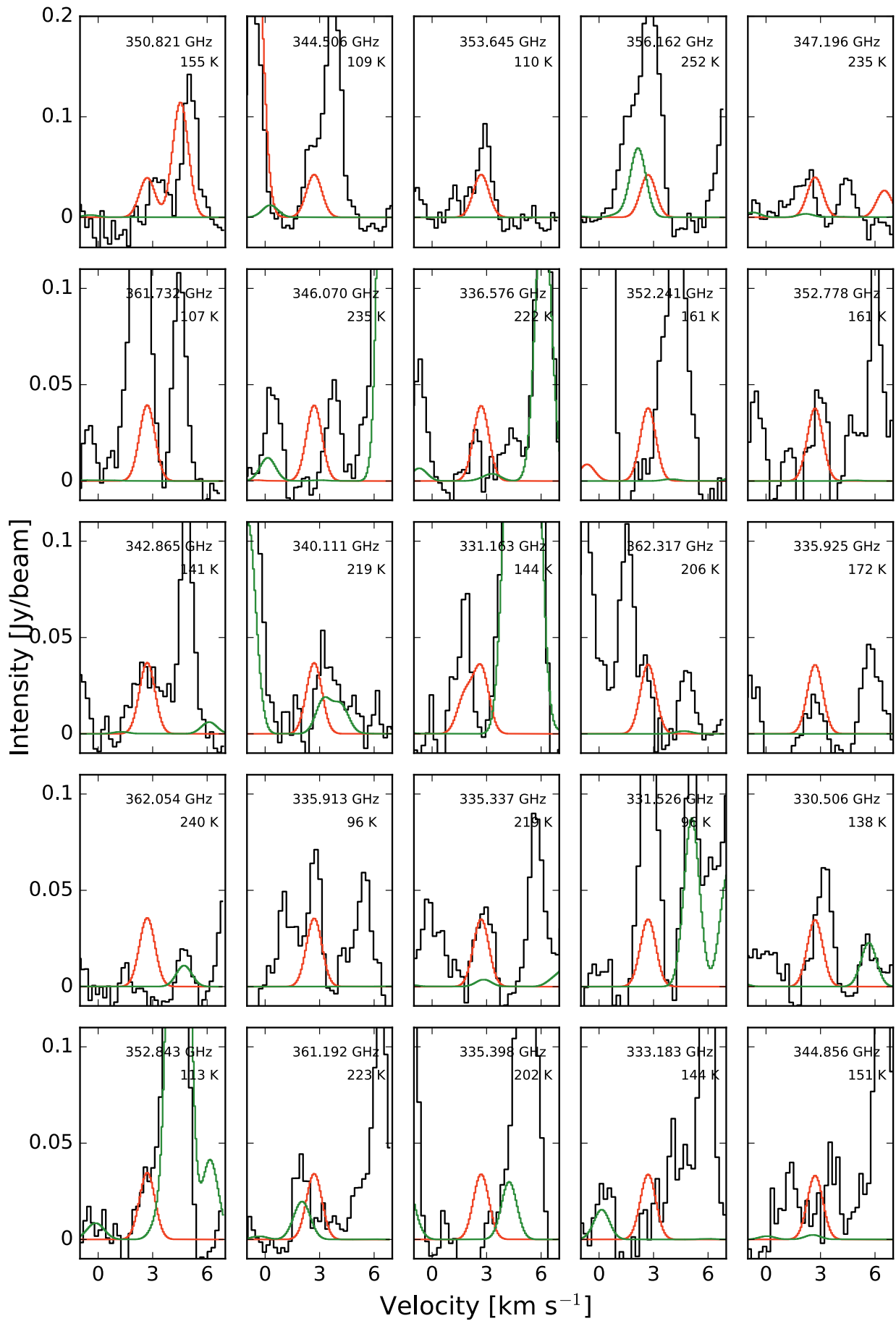


Fig. A.3. continued.

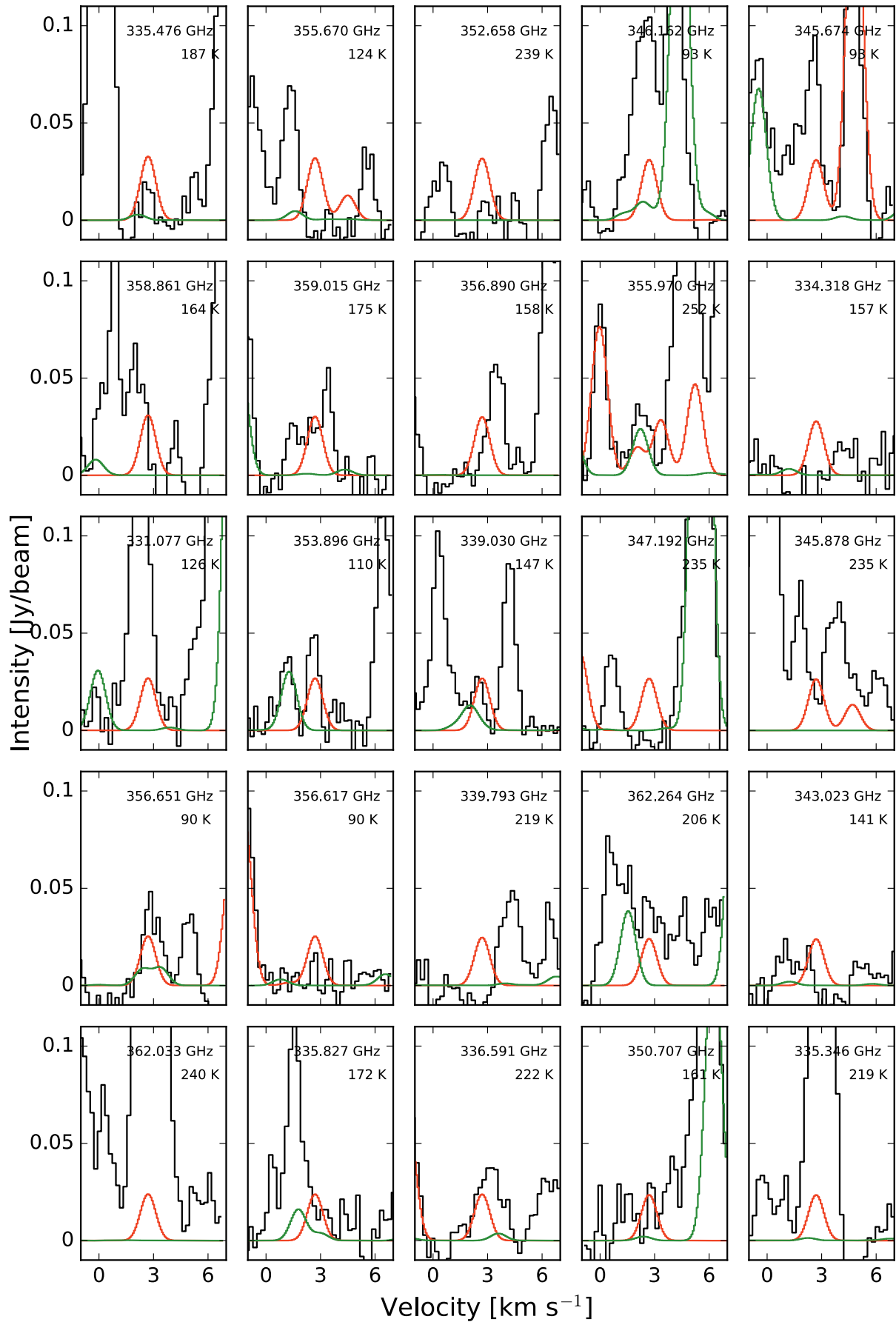


Fig. A.3. continued.

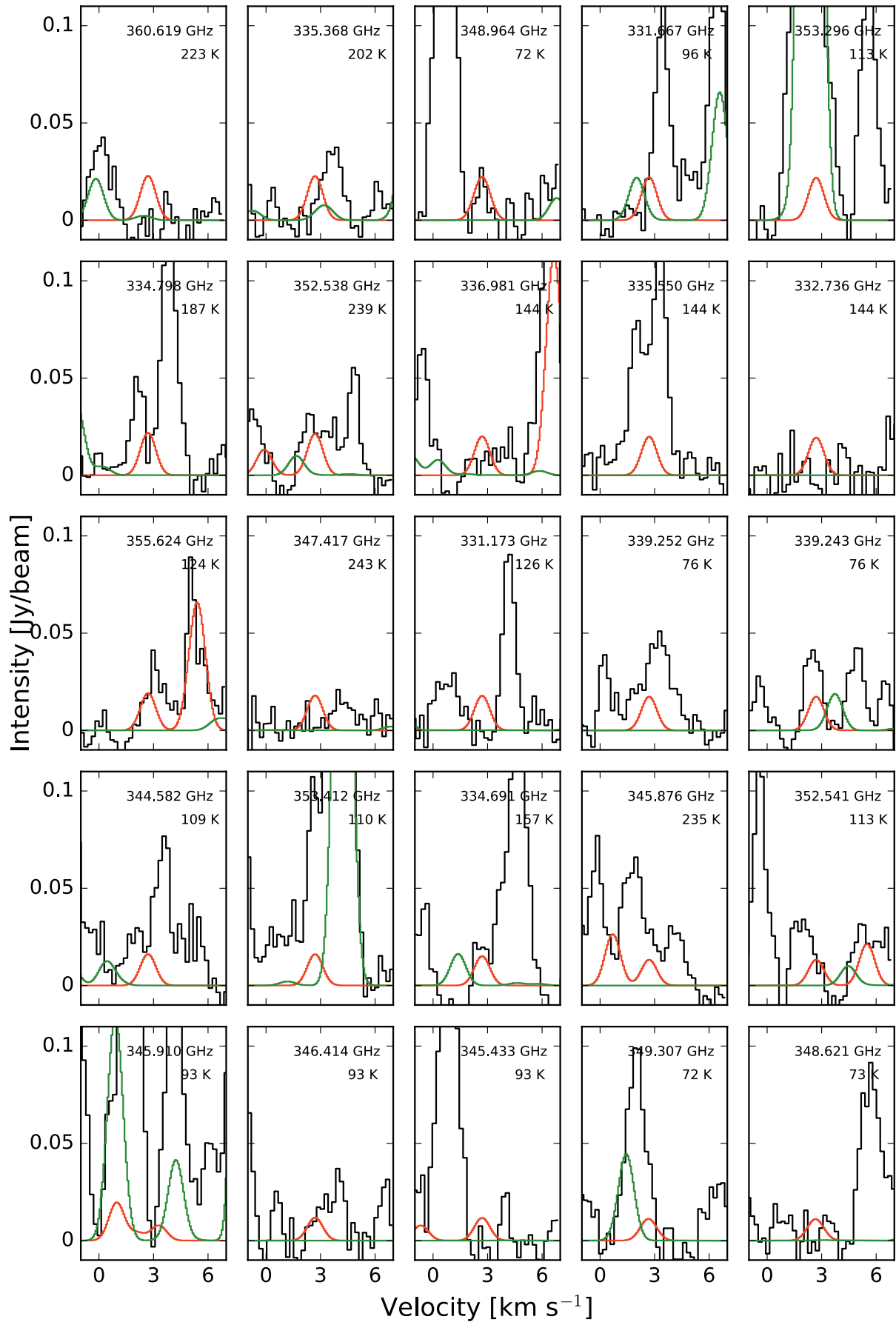


Fig. A.3. continued.

Appendix B: Detected lines

Table B.1. Catalog values for the detected propanal, ethylene oxide and acetone transitions and the integrated line strength of the synthetic spectrum.

Transition	Frequency [MHz]	E_{up} [K]	$\log_{10}(A_{\text{ul}})$ [s^{-1}]	τ	$\int_{\text{FWHM}} I \delta\nu$ [$\text{J beam}^{-1} \text{ km s}^{-1}$]	Detection level
Ethylene oxide ($\text{c-C}_2\text{H}_4\text{O}$)						
10 _{2,8} –9 _{3,7}	329 744.34	95	–3.3018	5.33e-01	0.248	69
10 _{3,8} –9 _{2,7}	329 748.33	95	–3.3019	3.20e-01	0.147	41
22 _{5,17} –22 _{4,18}	331 651.32	441	–3.7416	2.58e-02	0.064	18
22 _{6,17} –22 _{5,18}	331 651.32	441	–3.7416	1.55e-02	0.064	18
21 _{4,17} –21 _{3,18}	332 345.92	392	–3.8096	1.87e-02	0.034	10
21 _{5,17} –21 _{4,18}	332 345.92	392	–3.8097	3.12e-02	0.034	10
9 _{4,5} –8 _{5,4}	336 561.39	90	–3.5297	1.71e-01	0.156	44
11 _{7,5} –10 _{8,2}	338 295.96	138	–4.5667	2.15e-02	0.027	8
11 _{1,10} –10 _{2,9}	338 771.98	104	–3.1922	4.00e-01	0.428	120
11 _{2,10} –10 _{1,9}	338 771.98	104	–3.1921	6.66e-01	0.428	120
7 _{6,1} –6 _{5,2}	341 730.22	63	–3.3675	2.38e-01	0.229	64
9 _{5,5} –8 _{4,4}	345 688.32	90	–3.4727	3.09e-01	0.249	70
12 _{0,12} –11 _{1,11}	347 843.06	111	–3.1026	7.99e-01	0.542	151
12 _{1,12} –11 _{0,11}	347 843.10	111	–3.1027	4.79e-01	0.542	151
10 _{3,7} –9 _{4,6}	348 966.62	102	–3.3039	4.50e-01	0.273	76
10 _{4,7} –9 _{3,6}	349 099.82	102	–3.3033	2.70e-01	0.246	69
24 _{6,18} –24 _{5,19}	349 972.85	532	–3.6332	1.57e-02	0.034	10
24 _{7,18} –24 _{6,19}	349 972.85	532	–3.6333	9.45e-03	0.034	10
7 _{7,1} –6 _{6,0}	350 303.48	66	–3.1488	6.08e-01	0.404	113
7 _{7,0} –6 _{6,1}	350 644.59	66	–3.1479	3.65e-01	0.291	81
23 _{5,18} –23 _{4,19}	350 741.95	477	–3.6859	1.23e-02	0.026	7
23 _{6,18} –23 _{5,19}	350 741.95	477	–3.6859	2.06e-02	0.026	7
21 _{3,18} –21 _{2,19}	352 033.68	376	–3.8513	1.73e-02	0.031	9
21 _{4,18} –21 _{3,19}	352 033.68	376	–3.8513	2.88e-02	0.031	9
20 _{2,18} –20 _{1,19}	352 570.56	328	–3.9971	2.87e-02	0.046	13
20 _{3,18} –20 _{2,19}	352 570.56	328	–3.9971	1.72e-02	0.046	13
11 _{2,9} –10 _{3,8}	357 909.16	113	–3.1776	3.47e-01	0.371	104
11 _{3,9} –10 _{2,8}	357 909.70	113	–3.1776	5.78e-01	0.531	149
8 _{6,3} –7 _{5,2}	361 519.42	78	–3.4205	1.90e-01	0.194	54
Propanal ($\text{C}_2\text{H}_5\text{CHO}$)						
32 _{5,28} –31 _{5,27}	330 033.48	281	–3.2366	2.04e-02	0.013	4
32 _{4,28} –31 _{4,27}	330 572.90	281	–3.2344	2.04e-02	0.022	6
13 _{9,5} –12 _{8,4}	330 651.76	90	–3.3400	3.05e-02	0.042	12
13 _{9,4} –12 _{8,5}	330 651.76	90	–3.3400	3.05e-02	0.042	12
31 _{7,25} –30 _{7,24}	332 598.70	281	–3.2339	1.96e-02	0.012	3
31 _{5,26} –30 _{5,25}	332 939.34	273	–3.2271	2.12e-02	0.019	5
35 _{1,34} –34 _{2,33}	333 358.91	297	–3.2007	2.08e-02	0.089	25
35 _{2,34} –34 _{2,33}	333 358.92	297	–3.2123	2.03e-02	0.089	25
35 _{1,34} –34 _{1,33}	333 358.93	297	–3.2123	2.03e-02	0.089	25
35 _{2,34} –34 _{1,33}	333 358.95	297	–3.2007	2.08e-02	0.089	25
32 _{6,27} –31 _{6,26}	337 650.97	289	–3.2096	1.94e-02	0.015	4
20 _{6,14} –19 _{5,15}	338 096.89	127	–3.6845	1.50e-02	0.020	5
32 _{15,17} –31 _{15,16}	338 572.87	390	–3.2943	7.07e-03	0.013	4
32 _{15,18} –31 _{15,17}	338 572.87	390	–3.2943	7.07e-03	0.013	4
33 _{5,29} –32 _{5,28}	339 194.57	297	–3.2004	1.90e-02	0.020	6
33 _{4,29} –32 _{4,28}	339 547.63	297	–3.1990	1.90e-02	0.017	5
33 _{5,29} –32 _{4,28}	340 164.32	297	–3.3742	1.27e-02	0.020	6
14 _{9,6} –13 _{8,5}	341 151.22	97	–3.3271	3.00e-02	0.052	15
14 _{9,5} –13 _{8,6}	341 151.23	97	–3.3271	3.00e-02	0.052	15
35 _{2,33} –34 _{3,32}	341 277.32	309	–3.2188	1.73e-02	0.084	23
35 _{3,33} –34 _{3,32}	341 277.92	309	–3.1853	1.87e-02	0.084	23
35 _{2,33} –34 _{2,32}	341 278.36	309	–3.1853	1.87e-02	0.084	23
35 _{3,33} –34 _{2,32}	341 278.96	309	–3.2188	1.73e-02	0.084	23
20 _{5,15} –19 _{4,16}	341 279.21	122	–3.9480	8.36e-03	0.029	8
36 _{1,35} –35 _{2,34}	342 518.47	314	–3.1633	1.94e-02	0.057	16

Notes. Due to line contamination, the integrated line strength is given for the FWHM of the Gaussian function.

Table B.1. continued.

Transition	Frequency [MHz]	E_{up} [K]	$\log_{10}(A_{ul})$ [s ⁻¹]	τ	$\int_{FWHM} I \delta v$ [J beam ⁻¹ km s ⁻¹]	Detection level
36 _{2,35} –35 _{2,34}	342 518.47	314	–3.1767	1.88e-02	0.057	16
36 _{1,35} –35 _{1,34}	342 518.48	314	–3.1767	1.88e-02	0.057	16
36 _{2,35} –35 _{1,34}	342 518.49	314	–3.1633	1.94e-02	0.057	16
12 _{10,2} –11 _{9,3}	342 926.51	94	–3.2160	3.40e-02	0.072	20
12 _{10,3} –11 _{9,2}	342 926.51	94	–3.2160	3.40e-02	0.072	20
31 _{6,25} –30 _{6,24}	343 589.54	278	–3.1841	2.11e-02	0.027	8
31 _{7,24} –30 _{7,23}	343 711.33	283	–3.1880	2.01e-02	0.014	4
37 _{0,37} –36 _{1,36}	343 805.93	317	–3.1164	2.15e-02	0.072	20
37 _{1,37} –36 _{1,36}	343 805.93	317	–3.1679	1.91e-02	0.072	20
37 _{0,37} –36 _{0,36}	343 805.93	317	–3.1679	1.91e-02	0.072	20
37 _{1,37} –36 _{0,36}	343 805.93	317	–3.1164	2.15e-02	0.072	20
32 _{8,25} –31 _{8,24}	344 372.65	305	–3.1927	1.71e-02	0.024	7
34 _{4,30} –33 _{5,29}	347 948.63	314	–3.3326	1.20e-02	0.011	3
34 _{5,30} –33 _{5,29}	348 337.20	314	–3.1652	1.76e-02	0.017	5
35 _{4,32} –34 _{4,31}	349 293.49	321	–3.1583	1.74e-02	0.023	6
35 _{4,32} –34 _{3,31}	349 318.44	321	–3.2457	1.42e-02	0.021	6
36 _{2,34} –35 _{3,33}	350 430.33	326	–3.1805	1.61e-02	0.111	31
36 _{3,34} –35 _{3,33}	350 430.67	326	–3.1504	1.73e-02	0.111	31
36 _{2,34} –35 _{2,33}	350 430.92	326	–3.1504	1.73e-02	0.111	31
36 _{3,34} –35 _{2,33}	350 431.26	326	–3.1805	1.61e-02	0.111	31
37 _{1,36} –36 _{2,35}	351 676.10	331	–3.1270	1.80e-02	0.050	14
37 _{2,36} –36 _{2,35}	351 676.11	331	–3.1420	1.74e-02	0.050	14
37 _{1,36} –36 _{1,35}	351 676.11	331	–3.1420	1.74e-02	0.050	14
37 _{2,36} –36 _{1,35}	351 676.11	331	–3.1270	1.80e-02	0.050	14
38 _{0,38} –37 _{1,37}	352 965.05	334	–3.0815	1.98e-02	0.047	13
38 _{1,38} –37 _{1,37}	352 965.05	334	–3.1334	1.76e-02	0.047	13
38 _{0,38} –37 _{0,37}	352 965.05	334	–3.1334	1.76e-02	0.047	13
38 _{1,38} –37 _{0,37}	352 965.05	334	–3.0815	1.98e-02	0.047	13
32 _{6,26} –31 _{6,25}	353 148.80	295	–3.1484	1.95e-02	0.029	8
13 _{10,3} –12 _{9,4}	353 450.35	101	–3.2084	3.34e-02	0.060	17
33 _{9,25} –32 _{9,24}	354 555.43	331	–3.1598	1.47e-02	0.037	10
11 _{11,0} –10 _{10,1}	355 162.35	100	–3.0902	3.74e-02	0.083	23
11 _{11,1} –10 _{10,0}	355 162.35	100	–3.0902	3.74e-02	0.083	23
33 _{9,24} –32 _{9,23}	355 856.08	331	–3.1550	1.47e-02	0.023	7
34 _{6,29} –33 _{6,28}	356 384.80	323	–3.1379	1.67e-02	0.016	5
20 _{7,13} –19 _{6,14}	357 000.67	134	–3.5090	1.92e-02	0.032	9
35 _{5,31} –34 _{5,30}	357 467.93	331	–3.1310	1.63e-02	0.012	3
35 _{4,31} –34 _{4,30}	357 613.69	331	–3.1304	1.63e-02	0.016	5
34 _{5,29} –33 _{5,28}	358 305.47	323	–3.1306	1.68e-02	0.037	10
36 _{3,33} –35 _{3,32}	358 438.34	338	–3.1242	1.60e-02	0.015	4
37 _{2,35} –36 _{3,34}	359 581.63	343	–3.1434	1.50e-02	0.060	17
37 _{3,35} –36 _{3,34}	359 581.82	343	–3.1164	1.59e-02	0.060	17
37 _{2,35} –36 _{2,34}	359 581.97	343	–3.1164	1.59e-02	0.060	17
37 _{3,35} –36 _{2,34}	359 582.16	343	–3.1434	1.50e-02	0.060	17
18 _{8,10} –17 _{7,11}	359 812.79	122	–3.3969	2.43e-02	0.030	8
38 _{1,37} –37 _{2,36}	360 831.75	348	–3.0917	1.66e-02	0.059	16
38 _{2,37} –37 _{2,36}	360 831.75	348	–3.1082	1.60e-02	0.059	16
38 _{1,37} –37 _{1,36}	360 831.75	348	–3.1082	1.60e-02	0.059	16
38 _{2,37} –37 _{1,36}	360 831.75	348	–3.0917	1.66e-02	0.059	16
34 _{13,22} –33 _{13,21}	361 033.21	394	–3.1711	8.54e-03	0.028	8
34 _{13,21} –33 _{13,20}	361 033.31	394	–3.1711	8.54e-03	0.028	8
39 _{0,39} –38 _{1,38}	362 122.12	351	–3.0475	1.82e-02	0.067	19
39 _{0,39} –38 _{0,38}	362 122.12	351	–3.0999	1.61e-02	0.067	19
39 _{1,39} –38 _{0,38}	362 122.12	351	–3.0475	1.82e-02	0.067	19
39 _{1,39} –38 _{1,38}	362 122.12	351	–3.0999	1.61e-02	0.067	19
33 _{6,27} –32 _{6,26}	362 196.30	313	–3.1159	1.80e-02	0.019	5
Acetone (CH ₃ COCH ₃)						
26 _{8,18} –25 _{9,17} EA	329 228.06	244	–2.9657	3.38e-02	0.130	36
26 _{9,18} –25 _{8,17} EA	329 228.06	244	–2.9657	3.38e-02	0.130	36

Table B.1. continued.

Transition	Frequency [MHz]	E_{up} [K]	$\log_{10}(A_{\text{ul}})$ [s ⁻¹]	τ	$\int_{\text{FWHM}} I \delta v$ [J beam ⁻¹ km s ⁻¹]	Detection level
26 _{8,18} –25 _{9,17} AE	329 228.14	244	–2.9657	1.69e-02	0.130	36
26 _{9,18} –25 _{8,17} AE	329 228.14	244	–2.9657	5.07e-02	0.130	36
26 _{8,18} –25 _{9,17} EE	329 298.16	244	–2.9656	1.35e-01	0.178	50
26 _{9,18} –25 _{8,17} EE	329 298.16	244	–2.9656	1.35e-01	0.178	50
14 _{7,8} –13 _{4,9} AA	329 367.94	80	–4.0975	1.27e-02	0.118	33
26 _{8,18} –25 _{9,17} AA	329 368.09	244	–2.9654	5.07e-02	0.117	33
26 _{9,18} –25 _{8,17} AA	329 368.10	244	–2.9654	8.45e-02	0.117	33
27 _{7,20} –26 _{8,19} EA	330 250.07	252	–2.9233	3.60e-02	0.114	32
27 _{8,20} –26 _{7,19} EA	330 250.07	252	–2.9233	3.60e-02	0.114	32
27 _{7,20} –26 _{8,19} AE	330 250.13	252	–2.9233	5.40e-02	0.114	32
27 _{8,20} –26 _{7,19} AE	330 250.13	252	–2.9232	1.80e-02	0.114	32
51 _{13,38} –51 _{13,39} EE	330 250.15	875	–3.5999	2.36e-04	0.114	32
51 _{14,38} –51 _{13,39} EE	330 250.15	875	–3.2461	5.32e-04	0.114	32
51 _{13,38} –51 _{12,39} EE	330 250.15	875	–3.2461	5.32e-04	0.114	32
51 _{14,38} –51 _{12,39} EE	330 250.15	875	–3.5999	2.36e-04	0.114	32
27 _{7,20} –26 _{8,19} EE	330 314.39	252	–2.9231	1.44e-01	0.198	55
27 _{8,20} –26 _{7,19} EE	330 314.39	252	–2.9231	1.44e-01	0.198	55
27 _{7,20} –26 _{8,19} AA	330 378.56	252	–2.9230	9.00e-02	0.122	34
27 _{8,20} –26 _{7,19} AA	330 378.56	252	–2.9230	5.40e-02	0.122	34
17 _{15,3} –16 _{14,2} AE	330 506.31	138	–2.8918	3.06e-02	0.035	10
17 _{15,2} –16 _{14,3} AE	330 512.29	138	–2.8918	9.19e-02	0.038	11
17 _{15,3} –16 _{14,3} EA	330 549.33	138	–2.8919	6.13e-02	0.057	16
17 _{15,2} –16 _{14,2} EE	330 725.88	138	–2.8905	2.45e-01	0.207	58
17 _{15,3} –16 _{14,3} EE	330 765.02	138	–2.8906	2.45e-01	0.153	43
13 _{3,10} –12 _{2,11} EE	331 129.66	60	–4.7227	5.19e-03	0.015	4
13 _{4,10} –12 _{1,11} EE	331 129.71	60	–4.7227	5.19e-03	0.015	4
28 _{6,22} –27 _{7,21} EA	331 321.41	260	–2.8862	3.80e-02	0.148	41
28 _{7,22} –27 _{6,21} EA	331 321.41	260	–2.8862	3.80e-02	0.148	41
28 _{6,22} –27 _{7,21} AE	331 321.46	260	–2.8863	1.90e-02	0.148	41
28 _{7,22} –27 _{6,21} AE	331 321.46	260	–2.8863	5.70e-02	0.148	41
28 _{7,22} –27 _{7,21} EE	331 380.50	260	–3.0073	1.15e-01	0.191	53
28 _{6,22} –27 _{7,21} EE	331 380.50	260	–3.4997	3.70e-02	0.191	53
28 _{6,22} –27 _{6,21} EE	331 380.50	260	–3.0094	1.15e-01	0.191	53
28 _{7,22} –27 _{6,21} EE	331 380.50	260	–3.4932	3.76e-02	0.191	53
29 _{5,24} –28 _{5,23} EA	332 420.74	266	–2.8535	4.00e-02	0.116	33
29 _{6,24} –28 _{6,23} EA	332 420.74	266	–2.8535	4.00e-02	0.116	33
29 _{5,24} –28 _{5,23} AE	332 420.79	266	–2.8535	2.00e-02	0.116	33
29 _{6,24} –28 _{6,23} AE	332 420.79	266	–2.8535	6.00e-02	0.116	33
29 _{5,24} –28 _{5,23} EE	332 474.57	266	–3.4029	4.52e-02	0.185	52
29 _{5,24} –28 _{6,23} EE	332 474.57	266	–2.9972	1.15e-01	0.185	52
29 _{6,24} –28 _{6,23} EE	332 474.57	266	–3.4029	4.52e-02	0.185	52
29 _{6,24} –28 _{5,23} EE	332 474.57	266	–2.9972	1.15e-01	0.185	52
29 _{6,24} –28 _{6,23} AA	332 528.32	266	–2.8532	1.00e-01	0.125	35
29 _{5,24} –28 _{5,23} AA	332 528.32	266	–2.8532	6.00e-02	0.125	35
30 _{4,26} –29 _{5,25} EA	333 537.35	272	–2.8239	4.20e-02	0.139	39
30 _{5,26} –29 _{4,25} EA	333 537.35	272	–2.8239	4.20e-02	0.139	39
30 _{5,26} –29 _{5,25} AE	333 537.39	272	–2.8240	2.10e-02	0.139	39
30 _{4,26} –29 _{4,25} AE	333 537.39	272	–2.8240	6.30e-02	0.139	39
30 _{4,26} –29 _{4,25} EE	333 585.34	272	–4.7355	2.06e-03	0.235	66
30 _{5,26} –29 _{4,25} EE	333 585.34	272	–2.8291	1.66e-01	0.235	66
30 _{4,26} –29 _{5,25} EE	333 585.34	272	–2.8291	1.66e-01	0.235	66
30 _{5,26} –29 _{5,25} EE	333 585.34	272	–4.7355	2.06e-03	0.235	66
30 _{4,26} –29 _{5,25} AA	333 633.28	272	–2.8236	6.30e-02	0.170	48
30 _{5,26} –29 _{4,25} AA	333 633.28	272	–2.8237	1.05e-01	0.170	48
19 _{13,7} –18 _{12,6} AE	334 691.41	157	–3.2379	1.29e-02	0.018	5
31 _{3,28} –30 _{3,27} EE	334 706.67	277	–3.2332	6.39e-02	0.255	71
31 _{3,28} –30 _{4,27} EE	334 706.67	277	–2.9889	1.12e-01	0.255	71
31 _{4,28} –30 _{4,27} EE	334 706.67	277	–3.2332	6.39e-02	0.255	71
31 _{4,28} –30 _{3,27} EE	334 706.67	277	–2.9889	1.12e-01	0.255	71
31 _{3,28} –30 _{4,27} AA	334 747.64	277	–2.7968	1.10e-01	0.149	42

Table B.1. continued.

Transition	Frequency [MHz]	E_{up} [K]	$\log_{10}(A_{\text{ul}})$ [s ⁻¹]	τ	$\int_{FWHM} I \delta v$ [J beam ⁻¹ km s ⁻¹]	Detection level
31 _{3,28} -30 _{4,27} AA	334 747.64	277	-2.7968	1.10e-01	0.160	45
31 _{4,28} -30 _{3,27} AA	334 747.64	277	-2.7969	6.60e-02	0.149	42
31 _{4,28} -30 _{3,27} AA	334 747.64	277	-2.7969	6.60e-02	0.160	45
21 _{13,9} -20 _{12,8} EE	335 150.46	187	-3.3155	7.48e-02	0.059	16
23 _{12,11} -22 _{13,10} AE	335 336.65	219	-3.2138	3.00e-02	0.033	9
23 _{12,11} -22 _{13,10} EE	335 427.63	219	-3.2142	8.00e-02	0.087	24
22 _{13,10} -21 _{12,9} EE	335 617.32	202	-3.2655	7.73e-02	0.075	21
32 _{2,30} -31 _{3,29} EA	335 802.89	281	-2.7724	4.61e-02	0.167	47
32 _{3,30} -31 _{2,29} EA	335 802.89	281	-2.7724	4.61e-02	0.167	47
32 _{2,30} -31 _{2,29} AE	335 802.91	281	-2.7724	6.92e-02	0.167	47
32 _{3,30} -31 _{3,29} AE	335 802.91	281	-2.7724	2.31e-02	0.167	47
32 _{2,30} -31 _{3,29} EE	335 835.06	281	-3.1155	8.05e-02	0.219	61
32 _{2,30} -31 _{2,29} EE	335 835.06	281	-3.0035	1.04e-01	0.219	61
32 _{3,30} -31 _{3,29} EE	335 835.06	281	-3.0035	1.04e-01	0.219	61
32 _{3,30} -31 _{2,29} EE	335 835.06	281	-3.1155	8.05e-02	0.219	61
32 _{3,30} -31 _{3,29} AA	335 867.22	281	-2.7722	6.93e-02	0.156	44
32 _{2,30} -31 _{2,29} AA	335 867.22	281	-2.7722	1.15e-01	0.156	44
15 _{9,7} -14 _{6,8} EE	335 913.15	96	-3.8800	3.03e-02	0.049	14
20 _{13,8} -19 _{12,7} AE	335 925.12	172	-3.3067	3.07e-02	0.013	4
17 _{16,2} -16 _{15,1} AE	336 425.06	142	-2.8089	3.46e-02	0.137	38
17 _{16,1} -16 _{15,2} AE	336 425.21	142	-2.8089	1.04e-01	0.137	38
17 _{16,2} -16 _{15,2} EA	336 499.84	142	-2.8087	6.93e-02	0.116	32
23 _{13,10} -22 _{14,9} EE	336 595.46	222	-3.3730	5.35e-02	0.043	12
17 _{16,1} -16 _{15,1} EE	336 627.03	142	-2.8079	2.77e-01	0.267	75
20 _{13,8} -19 _{12,7} AA	336 659.82	172	-3.3026	5.14e-02	0.019	5
17 _{16,2} -16 _{15,2} EE	336 700.98	142	-2.8077	2.77e-01	0.220	61
24 _{11,13} -23 _{12,12} EE	336 848.82	230	-3.0930	9.95e-02	0.105	29
24 _{12,13} -23 _{11,12} EA	336 881.18	230	-3.0924	2.49e-02	0.036	10
24 _{12,13} -23 _{11,12} AE	336 882.02	230	-3.0924	3.73e-02	0.036	10
17 _{16,2} -16 _{15,1} AA	336 902.73	142	-2.8067	1.04e-01	0.224	62
17 _{16,1} -16 _{15,2} AA	336 902.88	142	-2.8067	1.74e-01	0.224	62
24 _{11,13} -23 _{12,12} AA	336 942.18	230	-3.0931	3.73e-02	0.053	15
33 _{1,32} -32 _{2,31} EA	336 947.69	285	-2.7496	4.84e-02	0.158	44
33 _{2,32} -32 _{1,31} EA	336 947.69	285	-2.7496	4.84e-02	0.158	44
33 _{2,32} -32 _{2,31} AE	336 947.69	285	-2.7496	7.26e-02	0.158	44
33 _{1,32} -32 _{1,31} AE	336 947.69	285	-2.7496	2.42e-02	0.158	44
33 _{1,32} -32 _{2,31} EE	336 968.39	285	-2.8961	1.29e-01	0.221	62
33 _{2,32} -32 _{2,31} EE	336 968.39	285	-3.1937	6.50e-02	0.221	62
33 _{1,32} -32 _{1,31} EE	336 968.39	285	-3.1937	6.50e-02	0.221	62
33 _{2,32} -32 _{1,31} EE	336 968.39	285	-2.8961	1.29e-01	0.221	62
24 _{12,13} -23 _{11,12} EE	336 976.82	230	-3.0925	9.95e-02	0.129	36
33 _{1,32} -32 _{2,31} AA	336 989.07	285	-2.7495	1.21e-01	0.187	52
33 _{2,32} -32 _{1,31} AA	336 989.07	285	-2.7495	7.27e-02	0.187	52
24 _{12,13} -23 _{11,12} AA	337 071.78	230	-3.0924	6.22e-02	0.084	23
25 _{10,15} -24 _{11,14} EA	337 243.77	241	-3.0202	2.80e-02	0.059	16
25 _{10,15} -24 _{11,14} AE	337 243.93	241	-3.0202	4.20e-02	0.087	24
25 _{11,15} -24 _{10,14} EA	337 245.60	241	-3.0202	2.80e-02	0.045	12
25 _{11,15} -24 _{10,14} AE	337 245.77	241	-3.0203	1.40e-02	0.045	12
25 _{10,15} -24 _{11,14} EE	337 325.28	241	-3.0202	1.12e-01	0.060	17
25 _{11,15} -24 _{10,14} EE	337 327.12	241	-3.0202	1.12e-01	0.060	17
25 _{10,15} -24 _{11,14} AA	337 406.52	241	-3.0201	7.00e-02	0.038	11
25 _{11,15} -24 _{10,14} AA	337 408.37	241	-3.0201	4.20e-02	0.038	11
26 _{9,17} -25 _{10,16} EA	338 044.46	251	-2.9640	3.05e-02	0.168	47
26 _{10,17} -25 _{9,16} EA	338 044.48	251	-2.9640	3.05e-02	0.168	47
26 _{9,17} -25 _{10,16} AE	338 044.57	251	-2.9640	1.52e-02	0.168	47
26 _{10,17} -25 _{9,16} AE	338 044.58	251	-2.9640	4.57e-02	0.168	47
34 _{0,34} -33 _{1,33} EE	338 105.31	288	-3.4554	3.46e-02	0.243	68
34 _{1,34} -33 _{1,33} EE	338 105.31	288	-2.7657	1.69e-01	0.243	68
34 _{0,34} -33 _{0,33} EE	338 105.31	288	-2.7657	1.69e-01	0.243	68
34 _{1,34} -33 _{0,33} EE	338 105.31	288	-3.4554	3.46e-02	0.243	68

Table B.1. continued.

Transition	Frequency [MHz]	E_{up} [K]	$\log_{10}(A_{\text{ul}})$ [s ⁻¹]	τ	$\int_{\text{FWHM}} I \delta v$ [J beam ⁻¹ km s ⁻¹]	Detection level
34 _{0,34} -33 _{0,33} AA	338 110.81	287	-2.7284	1.27e-01	0.197	55
34 _{1,34} -33 _{1,33} AA	338 110.81	287	-2.7283	7.65e-02	0.197	55
26 _{9,17} -25 _{10,16} EE	338 117.64	251	-2.9640	1.22e-01	0.210	59
26 _{10,17} -25 _{9,16} EE	338 117.66	251	-2.9640	1.22e-01	0.210	59
26 _{9,17} -25 _{10,16} AA	338 190.61	251	-2.9638	4.57e-02	0.114	32
26 _{10,17} -25 _{9,16} AA	338 190.62	251	-2.9638	7.61e-02	0.114	32
18 _{14,5} -17 _{13,5} EA	338 648.66	147	-3.0058	4.43e-02	0.030	8
18 _{14,4} -17 _{13,4} EE	338 833.86	147	-3.0148	1.73e-01	0.148	41
18 _{14,4} -17 _{13,5} AE	339 030.13	147	-2.9994	2.24e-02	0.018	5
27 _{8,19} -26 _{9,18} EE	339 069.60	260	-2.9174	1.30e-01	0.173	48
27 _{9,19} -26 _{8,18} EE	339 069.60	260	-2.9174	1.30e-01	0.173	48
27 _{8,19} -26 _{9,18} AA	339 136.45	260	-2.9173	8.13e-02	0.119	33
27 _{9,19} -26 _{8,18} AA	339 136.45	260	-2.9172	4.88e-02	0.119	33
14 _{5,9} -13 _{4,10} EE	339 242.67	76	-4.2327	1.44e-02	0.032	9
23 _{13,11} -22 _{12,10} EE	339 955.49	219	-3.1917	8.21e-02	0.078	22
28 _{7,21} -27 _{8,20} EA	340 038.58	269	-2.8776	3.44e-02	0.136	38
28 _{8,21} -27 _{7,20} EA	340 038.58	269	-2.8776	3.44e-02	0.136	38
28 _{7,21} -27 _{8,20} AE	340 038.65	269	-2.8777	1.72e-02	0.136	38
28 _{8,21} -27 _{7,20} AE	340 038.65	269	-2.8776	5.16e-02	0.136	38
28 _{7,21} -27 _{8,20} EE	340 100.55	269	-2.8776	1.37e-01	0.187	52
28 _{8,21} -27 _{7,20} EE	340 100.55	269	-2.8776	1.37e-01	0.187	52
28 _{7,21} -27 _{8,20} AA	340 162.36	269	-2.8774	5.16e-02	0.112	31
28 _{8,21} -27 _{7,20} AA	340 162.36	269	-2.8774	8.59e-02	0.112	31
29 _{7,23} -28 _{7,22} EA	341 116.83	276	-2.8426	3.61e-02	0.132	37
29 _{6,23} -28 _{6,22} EA	341 116.83	276	-2.8426	3.61e-02	0.132	37
29 _{6,23} -28 _{6,22} AE	341 116.89	276	-2.8426	1.81e-02	0.132	37
29 _{7,23} -28 _{7,22} AE	341 116.89	276	-2.8426	5.42e-02	0.132	37
29 _{7,23} -28 _{7,22} EE	341 174.15	276	-6.0035	9.97e-05	0.200	56
29 _{6,23} -28 _{7,22} EE	341 174.15	276	-2.8428	1.44e-01	0.200	56
29 _{6,23} -28 _{6,22} EE	341 174.15	276	-6.0035	9.97e-05	0.200	56
29 _{7,23} -28 _{6,22} EE	341 174.15	276	-2.8428	1.44e-01	0.200	56
29 _{6,23} -28 _{7,22} AA	341 231.36	276	-2.8423	9.03e-02	0.132	37
29 _{7,23} -28 _{6,22} AA	341 231.36	276	-2.8424	5.42e-02	0.132	37
44 _{5,39} -44 _{5,40} EE	341 950.48	562	-3.5251	3.21e-03	0.013	4
44 _{6,39} -44 _{5,40} EE	341 950.48	562	-4.1489	7.62e-04	0.013	4
44 _{5,39} -44 _{4,40} EE	341 950.48	562	-4.1489	7.62e-04	0.013	4
44 _{6,39} -44 _{4,40} EE	341 950.48	562	-3.5251	3.21e-03	0.013	4
30 _{6,25} -29 _{6,24} EA	342 219.92	283	-2.8113	3.78e-02	0.124	35
30 _{5,25} -29 _{5,24} EA	342 219.92	283	-2.8113	3.78e-02	0.124	35
30 _{5,25} -29 _{5,24} AE	342 219.97	283	-2.8113	5.67e-02	0.124	35
30 _{6,25} -29 _{6,24} AE	342 219.97	283	-2.8113	1.89e-02	0.124	35
30 _{5,25} -29 _{6,24} EE	342 272.48	283	-3.8339	1.43e-02	0.208	58
30 _{6,25} -29 _{6,24} EE	342 272.48	283	-2.8544	1.37e-01	0.208	58
30 _{5,25} -29 _{5,24} EE	342 272.48	283	-2.8544	1.37e-01	0.208	58
30 _{6,25} -29 _{5,24} EE	342 272.48	283	-3.8339	1.43e-02	0.208	58
17 _{17,1} -16 _{16,0} AE	342 300.57	147	-2.7347	3.83e-02	0.142	40
17 _{17,0} -16 _{16,1} AE	342 300.57	147	-2.7346	1.15e-01	0.142	40
30 _{5,25} -29 _{6,24} AA	342 324.94	283	-2.8110	5.67e-02	0.130	36
30 _{6,25} -29 _{5,24} AA	342 324.94	283	-2.8111	9.45e-02	0.130	36
17 _{17,1} -16 _{16,1} EA	342 410.64	147	-2.7343	7.67e-02	0.095	26
17 _{17,0} -16 _{16,0} EE	342 485.23	147	-2.7339	3.06e-01	0.269	75
17 _{17,1} -16 _{16,1} EE	342 594.89	147	-2.7335	3.07e-01	0.229	64
17 _{17,1} -16 _{16,0} AA	342 780.03	147	-2.7327	1.15e-01	0.227	63
17 _{17,0} -16 _{16,1} AA	342 780.04	147	-2.7328	1.92e-01	0.227	63
31 _{4,27} -30 _{5,26} EA	343 338.88	289	-2.7830	3.95e-02	0.142	40
31 _{5,27} -30 _{4,26} EA	343 338.88	289	-2.7830	3.95e-02	0.142	40
31 _{4,27} -30 _{4,26} AE	343 338.92	289	-2.7830	1.97e-02	0.142	40
31 _{5,27} -30 _{5,26} AE	343 338.92	289	-2.7830	5.92e-02	0.142	40
31 _{4,27} -30 _{5,26} AA	343 433.08	289	-2.7828	9.87e-02	0.172	48
31 _{5,27} -30 _{4,26} AA	343 433.08	289	-2.7828	5.92e-02	0.172	48

Table B.1. continued.

Transition	Frequency [MHz]	E_{up} [K]	$\log_{10}(A_{ul})$ [s ⁻¹]	τ	$\int_{FWHM} I \delta v$ [J beam ⁻¹ km s ⁻¹]	Detection level
32 _{3,29} -31 _{4,28} EA	344 468.95	294	-2.7572	4.12e-02	0.114	32
32 _{4,29} -31 _{3,28} EA	344 468.95	294	-2.7572	4.12e-02	0.114	32
32 _{4,29} -31 _{4,28} AE	344 468.98	294	-2.7572	2.06e-02	0.114	32
32 _{3,29} -31 _{3,28} AE	344 468.98	294	-2.7572	6.19e-02	0.114	32
32 _{3,29} -31 _{3,28} EE	344 509.42	294	-3.7739	1.52e-02	0.182	51
32 _{3,29} -31 _{4,28} EE	344 509.42	294	-2.7817	1.50e-01	0.182	51
32 _{4,29} -31 _{3,28} EE	344 509.42	294	-2.7817	1.50e-01	0.182	51
32 _{4,29} -31 _{4,28} EE	344 509.42	294	-3.7739	1.52e-02	0.182	51
32 _{3,29} -31 _{4,28} AA	344 549.87	294	-2.7569	6.19e-02	0.181	51
32 _{4,29} -31 _{3,28} AA	344 549.87	294	-2.7570	1.03e-01	0.181	51
18 _{15,3} -17 _{14,3} EE	345 037.50	151	-2.8914	2.16e-01	0.142	40
18 _{15,4} -17 _{14,4} EE	345 073.72	151	-2.8917	2.15e-01	0.210	59
33 _{3,31} -32 _{3,30} EA	345 607.71	298	-2.7333	4.31e-02	0.183	51
33 _{2,31} -32 _{2,30} EA	345 607.71	298	-2.7333	4.31e-02	0.183	51
33 _{3,31} -32 _{3,30} AE	345 607.74	298	-2.7334	6.46e-02	0.183	51
33 _{2,31} -32 _{2,30} AE	345 607.74	298	-2.7334	2.15e-02	0.183	51
33 _{2,31} -32 _{3,30} EE	345 639.62	298	-3.5454	2.48e-02	0.200	56
33 _{2,31} -32 _{2,30} EE	345 639.62	298	-2.7700	1.48e-01	0.200	56
33 _{3,31} -32 _{3,30} EE	345 639.62	298	-2.7700	1.48e-01	0.200	56
33 _{3,31} -32 _{2,30} EE	345 639.62	298	-3.5454	2.48e-02	0.200	56
33 _{2,31} -32 _{2,30} AA	345 671.52	298	-2.7332	6.47e-02	0.140	39
33 _{3,31} -32 _{3,30} AA	345 671.52	298	-2.7332	1.08e-01	0.140	39
25 _{11,14} -24 _{12,13} EA	346 346.12	247	-3.0311	2.48e-02	0.078	22
25 _{11,14} -24 _{12,13} AE	346 346.31	247	-3.0310	3.72e-02	0.078	22
25 _{12,14} -24 _{11,13} EA	346 374.84	247	-3.0309	2.48e-02	0.042	12
25 _{12,14} -24 _{11,13} AE	346 375.23	247	-3.0310	1.24e-02	0.042	12
25 _{11,14} -24 _{12,13} EE	346 432.88	247	-3.0311	9.90e-02	0.091	25
25 _{12,14} -24 _{11,13} EE	346 461.91	247	-3.0310	9.90e-02	0.068	19
25 _{11,14} -24 _{12,13} AA	346 519.31	247	-3.0311	6.19e-02	0.042	12
25 _{12,14} -24 _{11,13} AA	346 548.56	247	-3.0309	3.71e-02	0.067	19
34 _{1,33} -33 _{2,32} AA	346 795.27	301	-2.7111	6.78e-02	0.097	27
34 _{2,33} -33 _{1,32} AA	346 795.27	301	-2.7112	1.13e-01	0.097	27
26 _{10,16} -25 _{11,15} EA	346 941.16	258	-2.9664	2.73e-02	0.081	23
26 _{10,16} -25 _{11,15} AE	346 941.30	258	-2.9664	1.37e-02	0.081	23
26 _{11,16} -25 _{10,15} EA	346 941.51	258	-2.9664	2.73e-02	0.081	23
26 _{11,16} -25 _{10,15} AE	346 941.65	258	-2.9664	4.09e-02	0.081	23
26 _{10,16} -25 _{11,15} EE	347 017.52	258	-2.9663	1.09e-01	0.142	40
26 _{11,16} -25 _{10,15} EE	347 017.87	258	-2.9663	1.09e-01	0.142	40
26 _{10,16} -25 _{11,15} AA	347 093.62	258	-2.9662	4.09e-02	0.101	28
26 _{11,16} -25 _{10,15} AA	347 093.97	258	-2.9663	6.82e-02	0.101	28
24 _{13,12} -23 _{12,11} EE	347 309.14	235	-3.1182	8.51e-02	0.099	28
27 _{9,18} -26 _{10,17} EA	347 797.75	268	-2.9148	2.93e-02	0.138	39
27 _{10,18} -26 _{9,17} EA	347 797.75	268	-2.9148	2.93e-02	0.138	39
27 _{9,18} -26 _{10,17} AE	347 797.85	268	-2.9148	4.40e-02	0.138	39
27 _{10,18} -26 _{9,17} AE	347 797.85	268	-2.9148	1.47e-02	0.138	39
27 _{9,18} -26 _{10,17} EE	347 867.07	268	-2.9147	1.17e-01	0.186	52
27 _{10,18} -26 _{9,17} EE	347 867.08	268	-2.9147	1.17e-01	0.186	52
35 _{0,35} -34 _{1,34} AE	347 907.80	304	-2.6907	7.10e-02	0.130	36
35 _{1,35} -34 _{0,34} AE	347 907.80	304	-2.6907	2.37e-02	0.130	36
35 _{0,35} -34 _{1,34} EA	347 907.85	304	-2.6907	4.73e-02	0.130	36
35 _{1,35} -34 _{0,34} EA	347 907.85	304	-2.6907	4.73e-02	0.130	36
35 _{0,35} -34 _{1,34} AA	347 918.78	304	-2.6907	1.18e-01	0.133	37
35 _{1,35} -34 _{0,34} AA	347 918.78	304	-2.6907	7.11e-02	0.133	37
27 _{9,18} -26 _{10,17} AA	347 936.19	268	-2.9146	7.33e-02	0.085	24
27 _{10,18} -26 _{9,17} AA	347 936.20	268	-2.9145	4.40e-02	0.085	24
28 _{8,20} -27 _{9,19} EA	348 780.22	277	-2.8714	3.10e-02	0.092	26
28 _{9,20} -27 _{8,19} EA	348 780.22	277	-2.8714	3.10e-02	0.092	26
28 _{8,20} -27 _{9,19} AE	348 780.29	277	-2.8713	1.55e-02	0.092	26
28 _{9,20} -27 _{8,19} AE	348 780.29	277	-2.8714	4.65e-02	0.092	26
28 _{8,20} -27 _{9,19} EE	348 844.27	277	-2.8712	1.24e-01	0.144	40

Table B.1. continued.

Transition	Frequency [MHz]	E_{up} [K]	$\log_{10}(A_{\text{ul}})$ [s ⁻¹]	τ	$\int_{F_{\text{WHM}}} I \delta v$ [J beam ⁻¹ km s ⁻¹]	Detection level
28 _{9,20} –27 _{8,19} EE	348 844.27	277	–2.8712	1.24e-01	0.144	40
28 _{8,20} –27 _{9,19} AA	348 908.15	277	–2.8711	4.65e-02	0.097	27
28 _{9,20} –27 _{8,19} AA	348 908.15	277	–2.8711	7.76e-02	0.097	27
14 _{4,10} –13 _{3,11} EE	348 964.09	72	–4.4168	9.23e-03	0.014	4
14 _{5,10} –13 _{2,11} EE	348 964.42	72	–4.4168	9.23e-03	0.014	4
29 _{7,22} –28 _{8,21} EA	349 827.76	285	–2.8337	3.26e-02	0.120	34
29 _{8,22} –28 _{7,21} EA	349 827.76	285	–2.8337	3.26e-02	0.120	34
29 _{7,22} –28 _{8,21} AE	349 827.82	285	–2.8338	4.89e-02	0.120	34
29 _{8,22} –28 _{7,21} AE	349 827.82	285	–2.8338	1.63e-02	0.120	34
29 _{8,22} –28 _{8,21} EE	349 887.43	285	–2.8633	1.22e-01	0.150	42
29 _{7,22} –28 _{8,21} EE	349 887.43	285	–4.0142	8.60e-03	0.150	42
29 _{7,22} –28 _{7,21} EE	349 887.43	285	–2.8631	1.22e-01	0.150	42
29 _{8,22} –28 _{7,21} EE	349 887.43	285	–4.0172	8.54e-03	0.150	42
29 _{7,22} –28 _{8,21} AA	349 946.96	285	–2.8335	8.14e-02	0.100	28
29 _{8,22} –28 _{7,21} AA	349 946.96	285	–2.8334	4.89e-02	0.100	28
18 _{16,3} –17 _{15,2} AE	350 819.12	155	–2.8044	9.25e-02	0.070	19
18 _{16,2} –17 _{15,3} AE	350 821.27	155	–2.8044	3.08e-02	0.015	4
18 _{16,3} –17 _{15,3} EA	350 891.89	155	–2.8043	6.17e-02	0.047	13
30 _{6,24} –29 _{6,23} EA	350 911.96	293	–2.8004	3.40e-02	0.118	33
30 _{7,24} –29 _{7,23} EA	350 911.96	293	–2.8004	3.40e-02	0.118	33
30 _{6,24} –29 _{6,23} AE	350 912.01	293	–2.8004	5.10e-02	0.118	33
30 _{7,24} –29 _{7,23} AE	350 912.01	293	–2.8004	1.70e-02	0.118	33
30 _{6,24} –29 _{6,23} EE	350 967.54	293	–3.4934	2.76e-02	0.187	52
30 _{6,24} –29 _{7,23} EE	350 967.54	293	–2.8987	1.09e-01	0.187	52
30 _{7,24} –29 _{7,23} EE	350 967.54	293	–3.2594	4.73e-02	0.187	52
30 _{7,24} –29 _{6,23} EE	350 967.54	293	–2.9856	8.88e-02	0.187	52
18 _{16,2} –17 _{15,2} EE	351 012.48	155	–2.8033	2.47e-01	0.214	60
30 _{7,24} –29 _{7,23} AA	351 023.02	293	–2.8002	5.10e-02	0.111	31
30 _{6,24} –29 _{6,23} AA	351 023.02	293	–2.8002	8.51e-02	0.111	31
18 _{16,3} –17 _{15,3} EE	351 083.30	155	–2.8032	2.47e-01	0.182	51
18 _{16,3} –17 _{15,2} AA	351 274.14	155	–2.8021	1.55e-01	0.115	32
31 _{5,26} –30 _{5,25} EA	352 018.43	300	–2.7706	3.55e-02	0.135	38
31 _{6,26} –30 _{6,25} EA	352 018.43	300	–2.7706	3.55e-02	0.135	38
31 _{5,26} –30 _{6,25} AE	352 018.48	300	–2.7706	5.32e-02	0.135	38
31 _{6,26} –30 _{5,25} AE	352 018.48	300	–2.7705	1.77e-02	0.135	38
31 _{5,26} –30 _{6,25} EE	352 069.73	300	–5.6440	1.88e-04	0.187	52
31 _{5,26} –30 _{5,25} EE	352 069.73	300	–2.7671	1.42e-01	0.187	52
31 _{6,26} –30 _{6,25} EE	352 069.73	300	–2.7671	1.42e-01	0.187	52
31 _{6,26} –30 _{5,25} EE	352 069.73	300	–5.6440	1.88e-04	0.187	52
31 _{5,26} –30 _{5,25} AA	352 120.94	300	–2.7703	5.32e-02	0.136	38
31 _{6,26} –30 _{6,25} AA	352 120.94	300	–2.7703	8.87e-02	0.136	38
24 _{13,11} –23 _{14,10} EE	352 593.82	239	–3.2028	6.58e-02	0.080	22
19 _{14,6} –18 _{13,6} EA	352 777.63	161	–3.1271	2.93e-02	0.033	9
16 _{11,6} –15 _{8,7} EE	352 842.59	113	–3.8606	2.68e-02	0.035	10
16 _{11,6} –15 _{8,7} EE	352 842.59	113	–3.8606	2.68e-02	0.029	8
32 _{4,28} –31 _{5,27} EA	353 139.60	306	–2.7434	3.69e-02	0.116	32
32 _{5,28} –31 _{4,27} EA	353 139.60	306	–2.7434	3.69e-02	0.116	32
32 _{4,28} –31 _{4,27} AE	353 139.65	306	–2.7434	5.54e-02	0.116	32
32 _{5,28} –31 _{5,27} AE	353 139.65	306	–2.7433	1.85e-02	0.116	32
32 _{4,28} –31 _{4,27} EE	353 185.88	306	–2.7258	1.48e-01	0.185	52
32 _{5,28} –31 _{5,27} EE	353 185.88	306	–2.7258	1.48e-01	0.185	52
32 _{4,28} –31 _{5,27} AA	353 232.11	306	–2.7431	5.54e-02	0.114	32
32 _{5,28} –31 _{4,27} AA	353 232.11	306	–2.7432	9.23e-02	0.114	32
16 _{10,7} –15 _{7,8} EE	353 644.50	110	–3.7796	3.29e-02	0.061	17
16 _{10,7} –15 _{7,8} AA	353 896.48	110	–3.7790	2.06e-02	0.033	9
33 _{3,30} –32 _{4,29} EA	354 271.40	311	–2.7185	3.84e-02	0.171	48
33 _{4,30} –32 _{3,29} EA	354 271.40	311	–2.7185	3.84e-02	0.171	48
33 _{3,30} –32 _{3,29} AE	354 271.44	311	–2.7185	1.92e-02	0.171	48
33 _{4,30} –32 _{4,29} AE	354 271.44	311	–2.7185	5.76e-02	0.171	48
19 _{14,5} –18 _{13,6} AE	354 307.91	161	–3.0237	5.52e-02	0.033	9

Table B.1. continued.

Transition	Frequency [MHz]	E_{up} [K]	$\log_{10}(A_{\text{ul}})$ [s ⁻¹]	τ	$\int_{\text{FWHM}} I \delta v$ [J beam ⁻¹ km s ⁻¹]	Detection level
33 _{3,30} -32 _{4,29} EE	354 311.36	311	-3.6682	1.61e-02	0.269	75
33 _{3,30} -32 _{3,29} EE	354 311.36	311	-2.7358	1.38e-01	0.269	75
33 _{4,30} -32 _{4,29} EE	354 311.36	311	-2.7358	1.38e-01	0.269	75
33 _{4,30} -32 _{3,29} EE	354 311.36	311	-3.6682	1.61e-02	0.269	75
33 _{3,30} -32 _{4,29} AA	354 351.30	311	-2.7183	9.61e-02	0.176	49
33 _{4,30} -32 _{3,29} AA	354 351.30	311	-2.7183	5.77e-02	0.176	49
34 _{2,32} -33 _{3,31} EA	355 411.74	315	-2.6955	4.00e-02	0.129	36
34 _{3,32} -33 _{2,31} EA	355 411.74	315	-2.6955	4.00e-02	0.129	36
34 _{2,32} -33 _{2,31} AE	355 411.77	315	-2.6955	6.00e-02	0.129	36
34 _{3,32} -33 _{3,31} AE	355 411.77	315	-2.6955	2.00e-02	0.129	36
34 _{3,32} -33 _{3,31} EE	355 443.39	315	-2.6521	1.60e-01	0.201	56
34 _{2,32} -33 _{2,31} EE	355 443.39	315	-2.6521	1.60e-01	0.201	56
34 _{3,32} -33 _{3,31} AA	355 475.05	315	-2.6953	6.01e-02	0.239	67
34 _{2,32} -33 _{2,31} AA	355 475.05	315	-2.6953	1.00e-01	0.239	67
25 _{12,13} -24 _{13,12} AE	355 620.72	252	-3.0519	3.23e-02	0.053	15
25 _{12,13} -24 _{13,12} EA	355 621.08	252	-3.0519	2.15e-02	0.053	15
25 _{12,13} -24 _{13,12} EE	355 713.67	252	-3.0520	8.60e-02	0.092	26
25 _{12,13} -24 _{13,12} AA	355 806.17	252	-3.0520	5.37e-02	0.040	11
26 _{12,15} -25 _{11,14} EA	355 972.75	264	-2.9740	2.43e-02	0.064	18
26 _{12,15} -25 _{11,14} AE	355 972.99	264	-2.9740	3.64e-02	0.064	18
26 _{11,15} -25 _{12,14} EE	356 046.79	264	-2.9739	9.71e-02	0.110	31
26 _{12,15} -25 _{11,14} EE	356 052.97	264	-2.9739	9.71e-02	0.107	30
25 _{13,13} -24 _{12,12} EE	356 066.12	252	-3.0504	8.61e-02	0.124	35
26 _{12,15} -25 _{11,14} AA	356 132.86	264	-2.9739	6.07e-02	0.057	16
35 _{1,34} -34 _{1,33} EA	356 559.73	319	-2.6741	4.18e-02	0.127	35
35 _{2,34} -34 _{2,33} EA	356 559.73	319	-2.6741	4.18e-02	0.127	35
35 _{1,34} -34 _{1,33} AE	356 559.73	319	-2.6741	2.09e-02	0.127	35
35 _{2,34} -34 _{2,33} AE	356 559.73	319	-2.6740	6.27e-02	0.127	35
35 _{1,34} -34 _{2,33} EE	356 580.23	319	-2.6206	1.66e-01	0.196	55
35 _{2,34} -34 _{2,33} EE	356 580.23	319	-4.8932	8.88e-04	0.196	55
35 _{1,34} -34 _{1,33} EE	356 580.23	319	-4.8932	8.88e-04	0.196	55
35 _{2,34} -34 _{1,33} EE	356 580.23	319	-2.6206	1.66e-01	0.196	55
35 _{1,34} -34 _{2,33} AA	356 600.73	319	-2.6740	1.05e-01	0.128	36
35 _{2,34} -34 _{1,33} AA	356 600.73	319	-2.6740	6.28e-02	0.128	36
18 _{17,1} -17 _{16,1} EA	356 621.39	160	-2.7275	6.88e-02	0.065	18
27 _{10,17} -26 _{11,16} EA	356 658.41	275	-2.9156	2.63e-02	0.112	31
27 _{11,17} -26 _{10,16} EA	356 658.48	275	-2.9156	2.63e-02	0.112	31
27 _{10,17} -26 _{11,16} AE	356 658.54	275	-2.9156	3.95e-02	0.112	31
27 _{11,17} -26 _{10,16} AE	356 658.60	275	-2.9156	1.32e-02	0.112	31
18 _{17,2} -17 _{16,1} AE	356 727.49	159	-2.7272	1.03e-01	0.070	20
18 _{17,1} -17 _{16,2} AE	356 727.54	159	-2.7272	3.44e-02	0.070	20
27 _{10,17} -26 _{11,16} AA	356 801.31	275	-2.9153	6.58e-02	0.097	27
27 _{11,17} -26 _{10,16} AA	356 801.37	275	-2.9154	3.95e-02	0.097	27
18 _{17,2} -17 _{16,2} EA	356 833.46	159	-2.7269	6.89e-02	0.078	22
18 _{17,1} -17 _{16,1} EE	356 902.77	160	-2.7263	2.75e-01	0.193	54
18 _{17,2} -17 _{16,2} EE	357 008.08	159	-2.7261	2.76e-01	0.289	81
18 _{17,2} -17 _{16,1} AA	357 183.43	160	-2.7252	1.72e-01	0.225	63
18 _{17,1} -17 _{16,2} AA	357 183.48	160	-2.7253	1.03e-01	0.225	63
28 _{9,19} -27 _{10,18} EA	357 558.00	285	-2.8678	2.80e-02	0.106	30
28 _{10,19} -27 _{9,18} EA	357 558.01	285	-2.8678	2.80e-02	0.106	30
28 _{9,19} -27 _{10,18} AE	357 558.09	285	-2.8678	1.40e-02	0.106	30
28 _{10,19} -27 _{9,18} AE	357 558.09	285	-2.8678	4.20e-02	0.106	30
28 _{9,19} -27 _{10,18} EE	357 623.66	285	-2.8677	1.12e-01	0.182	51
28 _{10,19} -27 _{9,18} EE	357 623.66	285	-2.8677	1.12e-01	0.182	51
28 _{9,19} -27 _{10,18} AA	357 689.11	285	-2.8675	4.20e-02	0.127	35
28 _{10,19} -27 _{9,18} AA	357 689.11	285	-2.8676	6.99e-02	0.127	35
36 _{0,36} -35 _{0,35} AE	357 715.22	322	-2.6541	6.56e-02	0.154	43
36 _{1,36} -35 _{1,35} AE	357 715.22	322	-2.6541	2.19e-02	0.154	43
36 _{0,36} -35 _{1,35} EA	357 715.27	322	-2.6541	4.37e-02	0.154	43
36 _{1,36} -35 _{0,35} EA	357 715.27	322	-2.6541	4.37e-02	0.154	43

Table B.1. continued.

Transition	Frequency [MHz]	E_{up} [K]	$\log_{10}(A_{\text{ul}})$ [s ⁻¹]	τ	$\int_{FWHM} I \delta v$ [J beam ⁻¹ km s ⁻¹]	Detection level
36 _{0,36} -35 _{1,35} EE	357 720.70	321	-2.5866	1.75e-01	0.235	66
36 _{1,36} -35 _{1,35} EE	357 720.70	321	-5.6153	1.64e-04	0.235	66
36 _{1,36} -35 _{0,35} EE	357 720.70	321	-2.5866	1.75e-01	0.235	66
36 _{0,36} -35 _{0,35} EE	357 720.70	321	-5.6153	1.64e-04	0.235	66
36 _{0,36} -35 _{1,35} AA	357 726.06	321	-2.6541	6.57e-02	0.155	43
36 _{1,36} -35 _{0,35} AA	357 726.06	321	-2.6541	1.09e-01	0.155	43
29 _{8,21} -28 _{9,20} EA	358 560.03	294	-2.8271	2.94e-02	0.126	35
29 _{9,21} -28 _{8,20} EA	358 560.03	294	-2.8271	2.94e-02	0.126	35
29 _{8,21} -28 _{9,20} AE	358 560.10	294	-2.8271	4.41e-02	0.126	35
29 _{9,21} -28 _{8,20} AE	358 560.10	294	-2.8270	1.47e-02	0.126	35
29 _{8,21} -28 _{9,20} EE	358 621.21	294	-2.8269	1.18e-01	0.195	55
29 _{9,21} -28 _{8,20} EE	358 621.21	294	-2.8269	1.18e-01	0.195	55
29 _{8,21} -28 _{9,20} AA	358 682.23	294	-2.8268	7.34e-02	0.118	33
29 _{9,21} -28 _{8,20} AA	358 682.23	294	-2.8268	4.41e-02	0.118	33
19 _{15,5} -18 _{14,5} EA	359 063.67	164	-2.9024	4.61e-02	0.052	15
19 _{15,4} -18 _{14,4} EE	359 225.22	164	-2.9025	1.84e-01	0.159	44
19 _{15,5} -18 _{14,5} EE	359 266.93	164	-2.9031	1.84e-01	0.142	40
30 _{8,23} -29 _{8,22} EA	359 617.24	303	-2.7914	3.07e-02	0.119	33
30 _{7,23} -29 _{7,22} EA	359 617.24	303	-2.7914	3.07e-02	0.119	33
30 _{7,23} -29 _{8,22} AE	359 617.31	303	-2.7914	1.53e-02	0.119	33
30 _{8,23} -29 _{7,22} AE	359 617.31	303	-2.7914	4.60e-02	0.119	33
30 _{7,23} -29 _{8,22} EE	359 674.69	303	-4.9449	8.61e-04	0.163	45
30 _{8,23} -29 _{8,22} EE	359 674.69	303	-2.7943	1.22e-01	0.163	45
30 _{8,23} -29 _{7,22} EE	359 674.69	303	-4.9449	8.61e-04	0.163	45
30 _{7,23} -29 _{7,22} EE	359 674.69	303	-2.7943	1.22e-01	0.163	45
30 _{8,23} -29 _{8,22} AA	359 731.98	303	-2.7912	4.60e-02	0.100	28
30 _{8,23} -29 _{8,22} AA	359 731.98	303	-2.7912	4.60e-02	0.102	28
30 _{7,23} -29 _{7,22} AA	359 731.98	303	-2.7911	7.67e-02	0.100	28
30 _{7,23} -29 _{7,22} AA	359 731.98	303	-2.7911	7.67e-02	0.102	28
31 _{6,25} -30 _{7,24} EA	360 706.63	310	-2.7597	3.19e-02	0.152	42
31 _{7,25} -30 _{6,24} EA	360 706.63	310	-2.7597	3.19e-02	0.152	42
31 _{6,25} -30 _{7,24} AE	360 706.68	310	-2.7597	4.78e-02	0.152	42
31 _{7,25} -30 _{6,24} AE	360 706.68	310	-2.7597	1.59e-02	0.152	42
31 _{7,25} -30 _{7,24} EE	360 760.53	310	-2.7647	1.25e-01	0.175	49
31 _{6,25} -30 _{7,24} EE	360 760.53	310	-4.4450	2.61e-03	0.175	49
31 _{6,25} -30 _{6,24} EE	360 760.53	310	-2.7559	1.27e-01	0.175	49
31 _{7,25} -30 _{6,24} EE	360 760.53	310	-6.1629	4.99e-05	0.175	49
31 _{6,25} -30 _{6,24} AA	360 814.30	310	-2.7595	4.78e-02	0.097	27
31 _{7,25} -30 _{7,24} AA	360 814.30	310	-2.7594	7.97e-02	0.097	27
23 _{14,10} -22 _{13,9} EE	360 915.54	223	-3.2141	6.73e-02	0.088	25
32 _{6,27} -31 _{6,26} EA	361 816.20	317	-2.7310	3.31e-02	0.155	43
32 _{5,27} -31 _{5,26} EA	361 816.20	317	-2.7310	3.31e-02	0.155	43
32 _{5,27} -31 _{5,26} AE	361 816.25	317	-2.7310	4.96e-02	0.155	43
32 _{6,27} -31 _{6,26} AE	361 816.25	317	-2.7311	1.65e-02	0.155	43
32 _{5,27} -31 _{6,26} EE	361 866.27	317	-2.7219	1.30e-01	0.204	57
32 _{6,27} -31 _{6,26} EE	361 866.27	317	-4.4333	2.52e-03	0.204	57
32 _{5,27} -31 _{5,26} EE	361 866.27	317	-4.4333	2.52e-03	0.204	57
32 _{6,27} -31 _{5,26} EE	361 866.27	317	-2.7219	1.30e-01	0.204	57
32 _{5,27} -31 _{6,26} AA	361 916.24	317	-2.7308	4.96e-02	0.133	37
32 _{6,27} -31 _{5,26} AA	361 916.24	317	-2.7308	8.27e-02	0.133	37
24 _{14,11} -23 _{13,10} EE	362 230.43	240	-3.1534	6.99e-02	0.063	18
18 _{18,0} -17 _{17,0} EA	362 458.25	164	-2.6580	7.52e-02	0.061	17
18 _{18,1} -17 _{17,0} AE	362 600.03	164	-2.6576	1.13e-01	0.154	43
18 _{18,0} -17 _{17,1} AE	362 600.03	164	-2.6576	3.76e-02	0.154	43
18 _{18,1} -17 _{17,1}	362 741.13	164	-2.6571	7.54e-02	0.173	48
18 _{18,0} -17 _{17,0} EE	362 755.32	164	-2.6569	3.01e-01	0.239	67
16 _{9,8} -15 _{6,9} EA	362 811.49	107	-3.8228	7.25e-03	0.019	5

Appendix C: Acetone lines with high K_a and low K_c quantum numbers**Table C.1.** Acetone lines with high K_a and low K_c quantum numbers

Transition	Predicted frequency [MHz]
$19_{13,7}-18_{12,6}$ EE	334 948.01
$18_{13,5}-17_{12,6}$ EE	336 133.79
$18_{14,5}-17_{13,4}$ AE	338 242.61
$18_{14,4}-17_{13,4}$ EA	338 625.87
$18_{14,4}-17_{13,5}$ AA	339 459.74
$18_{12,6}-17_{11,7}$ EE	342 896.39
$18_{15,3}-17_{14,3}$ EA	344 793.57
$19_{14,6}-18_{13,5}$ EE	350 205.27
$19_{14,6}-18_{13,5}$ AA	351 215.21
$19_{14,6}-18_{13,6}$ EE	353 155.67
$19_{14,5}-18_{13,6}$ AA	354 673.02
$19_{14,5}-18_{13,6}$ EE	355 248.54
$19_{13,6}-18_{12,7}$ AA	356 644.96
$19_{13,6}-18_{12,7}$ EE	356 675.20
$19_{15,4}-18_{14,5}$ AE	359 197.90
$19_{15,5}-18_{14,4}$ AA	359 301.10
$20_{14,7}-19_{13,6}$ EE	359 843.80
$20_{14,7}-19_{13,6}$ AA	360 338.51

Notes. These acetone lines appear missing or shifted when comparing the synthetic spectrum with the observed spectrum. This could be due to perturbations by interactions between the (high K_a , low K_c) levels and the levels from the lowest torsional excited states (Groner et al. 2002).