

# A deep search for large complex organic species toward IRAS16293-2422 B at 3 mm with ALMA

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## ABSTRACT

**Context.** Complex organic molecules (COMs) have been detected ubiquitously in protostellar systems. However, at shorter wavelengths (~0.8 mm), it is generally more difficult to detect larger molecules than at longer wavelengths (~3 mm) because of the increase in millimeter dust opacity, line confusion, and unfavorable partition function.

**Aims.** We aim to search for large molecules (more than eight atoms) in the Atacama Large Millimeter/submillimeter Array (ALMA) Band 3 spectrum of IRAS 16293-2422 B. In particular, the goal is to quantify the usability of ALMA Band 3 for molecular line surveys in comparison to similar studies at shorter wavelengths.

**Methods.** We used deep ALMA Band 3 observations of IRAS 16293-2422 B to search for more than 70 molecules and identified as many lines as possible in the spectrum. The spectral settings were set to specifically target three-carbon species such as *i*- and *n*-propanol and glycerol, the next step after glycolaldehyde and ethylene glycol in the hydrogenation of CO. We then derived the column densities and excitation temperatures of the detected species and compared the ratios with respect to methanol between Band 3 (~3 mm) and Band 7 (~1 mm, Protostellar Interferometric Line Survey) observations of this source to examine the effect of the dust optical depth.

**Results.** We identified lines of 31 molecules including many oxygen-bearing COMs such as CH<sub>3</sub>OH, CH<sub>2</sub>OHCHO, CH<sub>3</sub>CH<sub>2</sub>OH, and *c*-C<sub>2</sub>H<sub>4</sub>O and a few nitrogen- and sulfur-bearing ones such as HOCH<sub>2</sub>CN and CH<sub>3</sub>SH. The largest detected molecules are *gGg*-(CH<sub>2</sub>OH)<sub>2</sub> and CH<sub>3</sub>COCH<sub>3</sub>. We did not detect glycerol or *i*- and *n*-propanol, but we do provide upper limits for them which are in line with previous laboratory and observational studies. The line density in Band 3 is only ~2.5 times lower in frequency space than in Band 7. From the detected lines in Band 3 at a ≥ 6σ level, ~25 – 30% of them could not be identified indicating the need for more laboratory data of rotational spectra. We find similar column densities and column density ratios of COMs (within a factor ~2) between Band 3 and Band 7.

**Conclusions.** The effect of the dust optical depth for IRAS 16293-2422 B at an off-source location on column densities and column density ratios is minimal. Moreover, for warm protostars, long wavelength spectra (~3 mm) are not only crowded and complex, but they also take significantly longer integration times than shorter wavelength observations (~0.8 mm) to reach the same sensitivity limit. The 3 mm search has not yet resulted in the detection of larger and more complex molecules in warm sources. A full deep ALMA Band 2 – 3 (i.e., ~3 – 4 mm wavelengths) survey is needed to assess whether low frequency data have the potential to reveal more complex molecules in warm sources.

**Key words.** Astrochemistry – Stars: low-mass – Stars: protostars – ISM: abundances – ISM: molecules

## 1. Introduction

In the interstellar medium (ISM) complex organic molecules (COMs), defined as species with at least six atoms containing carbon (Herbst & van Dishoeck 2009), are particularly prominent in the protostellar phase. Although other phases of star formation such as the prestellar phase (e.g., Bacmann et al. 2012; Jiménez-Serra et al. 2016; McGuire et al. 2020; Scibelli & Shirley 2020) and the later protoplanetary disk phase (Öberg et al. 2015; Walsh et al. 2016; Booth et al. 2021; Brunken et al. 2022) show detections of these species, COMs are more easily detectable in the line-rich protostellar envelopes due to their higher temperatures (e.g., Blake et al. 1987; Belloche et al. 2013; Bergner et al. 2017; van Gelder et al. 2020; Nazari et al. 2021; Yang et al. 2021; McGuire 2022; Bianchi et al. 2022; Hsu et al. 2022).

Many COMs, including species with more than eight atoms, are expected to form in ices under laboratory conditions (ethanol – CH<sub>3</sub>CH<sub>2</sub>OH, Öberg et al. 2009; Chuang et al. 2020; Fedoseev et al. 2022; aminomethanol – NH<sub>2</sub>CH<sub>2</sub>OH, Theulé et al. 2013; glycerol – HOCH<sub>2</sub>CH(OH)CH<sub>2</sub>OH, Fedoseev et al. 2017; 1-

propanol – CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>OH, Qasim et al. 2019a,b; glycine – NH<sub>2</sub>CH<sub>2</sub>COOH, Ioppolo et al. 2021). However, there is a lot of debate regarding the ice or gas-phase formation of particular COMs (e.g., Ceccarelli et al. 2022). Two examples of these species are formamide (NH<sub>2</sub>CHO) and acetaldehyde (CH<sub>3</sub>CHO) for which both gas and ice formation pathways are suggested (e.g., Jones et al. 2011; Barone et al. 2015; Vazart et al. 2020; Chuang et al. 2020, 2021, 2022; Fedoseev et al. 2022; Garrod et al. 2022). To obtain clues as to the formation mechanism of COMs from an observational perspective, it is possible to search for the solid state signatures of COMs in ices (Schutte et al. 1999; Öberg et al. 2011) with telescopes such as the *James Webb Space Telescope* (Yang et al. 2022; McClure et al. 2023; Rocha et al. in prep.) using laboratory spectra available from, for example, the Leiden Ice Database for Astrochemistry (Rocha et al. 2022) and to examine the gas-phase correlations between different COMs in large samples of sources (Belloche et al. 2020; Coletta et al. 2020; Jørgensen et al. 2020; Nazari et al. 2022a; Taniguchi et al. 2023; Chen et al. 2023). However, observations and models show that physical effects such as the source structure or dust optical depth could affect the snowline locations,

gas-phase emission, and column density correlations of simple and complex molecules (Jørgensen et al. 2002; Persson et al. 2016; De Simone et al. 2020; Nazari et al. 2022b; Murillo et al. 2022a; Nazari et al. 2023a,b). Hence, interpretations of COM formation routes based on gas-phase observations can be affected by these physical factors. For example, an anticorrelation between column densities of two species (or a large scatter in the column density ratios) could have a physical origin rather than a chemical origin.

Among the low-mass protostars, the IRAS16293-2422 (IRAS16293 hereafter) triple protostellar system (Wootten 1989; Maureira et al. 2020) is one of the closest protostars, and one of the richest and most well-studied objects from a chemical perspective. The first detection of methanol (CH<sub>3</sub>OH; the simplest COM) toward a low-mass protostar was carried out by van Dishoeck et al. (1995) for this system. Since then, its chemistry and in particular the COMs in this system have been studied in more detail (Cazaux et al. 2003; Butner et al. 2007; Bisschop et al. 2008; Ceccarelli et al. 2010; Jørgensen et al. 2011; Jørgensen et al. 2012; Kahane et al. 2013; Jaber et al. 2014). More recently, the Protostellar Interferometric Line Survey (PILS; Jørgensen et al. 2016) studied IRAS16293 in Band 7 (~329.147 – 362.896 GHz) of the Atacama Large Millimeter/submillimeter Array (ALMA). This survey detected many COMs for the first time in the ISM, adding further information on complexity in space (Coutens et al. 2016; Lykke et al. 2017; Calcutt et al. 2018a; Jørgensen et al. 2018; Manigand et al. 2019; Manigand et al. 2021; Coutens et al. 2022).

However, a limitation of higher-frequency observations of ALMA (~330 GHz) is the higher degree of line blending. The reason is that for observations probing the same gas, the line width – although constant in velocity space – increases in frequency space (Jørgensen et al. 2020). Therefore, the detection of larger COMs with more than eight atoms, which have relatively weak lines, is expected to be easier at lower frequencies. Moreover, the heavier molecules have their Boltzmann distribution peak at lower frequencies than the lighter molecules at the same excitation temperature, and thus their lines are stronger at lower frequencies and they are more easily detected at long wavelength observations. On the other hand, the Boltzmann peak moves to the higher frequencies for higher temperatures (see Fig. 2 of Herbst & van Dishoeck 2009). Therefore, if the large molecules are thermally sublimated in the inner hot regions around the protostar (tracing warm or hot regions), it is difficult to observe these larger species even at low frequencies (although favored), unless the data are sensitive enough, which can be achieved at the expense of the angular resolution and longer integration times. The combination of the increase in line width in frequency space and the Boltzmann distribution peak of the lighter molecules being at higher frequencies also lead to spectra being more crowded, and thus it is more difficult to detect large molecules at high frequencies.

Moreover, dust optical depth effects could be an important issue at higher-frequency ALMA Bands 6 (~240 GHz) and 7 (~330 GHz). This is because of the larger dust opacity of ~1 mm-sized grains at shorter wavelengths (i.e., higher frequencies). For example, López-Sepulcre et al. (2017) found that NGC 1333 IRAS 4A1 in Perseus does not host any COMs when searched for with ALMA and the Plateau de Bure Interferometer. However, later, De Simone et al. (2020) detected methanol around this source at longer wavelengths with the Very Large Array (VLA). Another example is the ring-shaped structure of methanol around the dust continuum in the massive protostellar system 693050 (also known as G301.1364-00.2249) observed

by van Gelder et al. (2022b) at ~220 GHz with ALMA, which indicates dust attenuation on-source.

For this work, we used the deep Band 3 ALMA observations of IRAS16293 B to search for larger species (more than eight atoms). This dataset was specifically optimized to hunt for molecules such as glycerol and *i*- and *n*-propanol. Although the main aim is to specifically hunt for large molecules, we identified as many molecules as possible from the Cologne Database for Molecular Spectroscopy (CDMS; Müller et al. 2001; Müller et al. 2005) and the Jet Propulsion Laboratory database (JPL; Pickett et al. 1998) in our data. We fit the spectrum to derive the column densities and excitation temperatures of the detected species and we compared our results with those of PILS in Band 7. In particular, we examined whether dust attenuation is important for column densities and their ratios with respect to methanol (typically used as a reference species).

The paper is structured such that the observations are explained in Sect. 2. The results including the detected species and their column densities and excitation temperatures are given in Sect. 3. We discuss our findings, in particular the comparison with the PILS results in Sect. 4. Finally, we present our conclusions in Sect. 5.

## 2. Observations and methods

### 2.1. Data

This paper uses the data of IRAS16293 B taken with ALMA in Band 3 (project code: 2017.1.00518.S; PI: E. F. van Dishoeck). For more information on the data calibration, reduction, and imaging, as well as the first results on the gas accretion flow in the IRAS16293 system, readers can refer to Murillo et al. (2022b); here we give a brief description of the data. We used the data with the configuration C43-4, which were calibrated with the CASA pipeline (McMullin et al. 2007) and then self-calibrated with CASA. Continuum subtraction was done on the self-calibrated image datacubes using STATCONT (Sánchez-Monge et al. 2018).

The data have an angular resolution of ~0.9'' × 0.7'', which is larger than that of PILS (~0.5''). The frequency ranges covered were ~90.59 – 91.41 GHz (continuum), ~93.14 – 93.20 GHz, and ~103.28 – 103.52 GHz. After conversion of the flux to brightness temperature, the rms found from line-free regions in each spectral window was ~0.1 K, ~0.3 K, and 0.2 K (comparable to PILS), respectively, following a 171.7 minute on-source integration time. The spectral resolution was 0.805 km s<sup>-1</sup>, 0.049 km s<sup>-1</sup>, and 0.088 km s<sup>-1</sup>. Given that the lines have a full width at half maximum (FWHM) of ~1 – 2 km s<sup>-1</sup>, some lines are not fully resolved in the continuum window. The frequency range was optimized to cover transitions of larger species such as glycerol as well as *i*- and *n*-propanol. It also serendipitously covered transitions from other oxygen- and nitrogen-bearing COMs including glycolaldehyde (CH<sub>2</sub>OHCHO), propanal (g-C<sub>2</sub>H<sub>5</sub>CHO), and glycolonitrile (HOCH<sub>2</sub>CN). The spectrum of IRAS16293 B (Fig. 1) was extracted from the same 0.5'' offset position from the continuum peak of B that was used in many of the works from ALMA-PILS ( $\alpha_{J2000} = 16^{\text{h}}32^{\text{m}}22^{\text{s}}.58$  and  $\delta_{J2000} = -24^{\circ}28'32.8''$ , Coutens et al. 2016; Jørgensen et al. 2018; Calcutt et al. 2018b). Maps of a few common species tracing cold gas structures are presented in Murillo et al. (2022b).

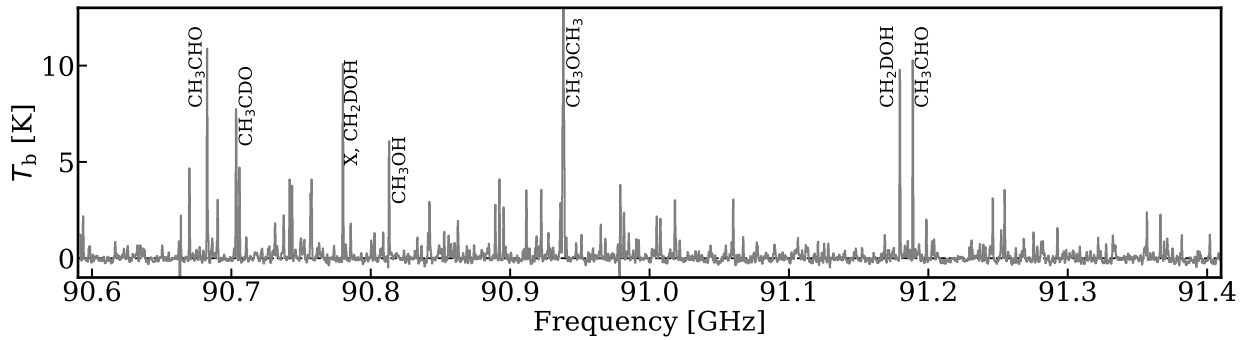


Fig. 1: Spectrum of IRAS16293 B Band 3 data for the continuum window. A few strong lines are highlighted; for the full line identification and fitting, readers can refer to Fig. B.1. We note that "X" indicates a line that has not been identified yet and that was not (fully) fitted with the considered molecules for this work. The spectrum of IRAS16293 B is line rich even at ALMA Band 3 wavelengths ( $\sim 3$  mm).

## 163 2.2. Spectral modeling

164 For this work, we identified as many molecules as possible using  
 165 the CASSIS<sup>1</sup> spectral analysis tool (Vastel et al. 2015). We  
 166 consider a molecule as detected if it has at least three lines at  
 167 a peak of the  $\geq 3\sigma$  level. We also report column densities of  
 168 the molecules that have one or two detected lines without any  
 169 overprediction of the emission in the spectrum. These column  
 170 densities are only tentative and not as robust as those found for  
 171 molecules with many detected lines because of the limited fre-  
 172 quency coverage, but they should be reliable for the most abun-  
 173 dant and common molecules such as <sup>13</sup>CH<sub>3</sub>OH. Using CAS-  
 174 SIS, we fit for the identified molecules. In the fitting procedure,  
 175 the spectrum was considered as a whole; and all the lines of  
 176 a molecule were fitted simultaneously assuming local thermo-  
 177 dynamic equilibrium (LTE) conditions. The fitting followed a  
 178 similar procedure as the fit-by-eye method used in Nazari et al.  
 179 (2022a). This includes varying the column densities ( $N$ ) and  
 180 excitation temperatures ( $T_{\text{ex}}$ ) in the LTE models to produce a  
 181 synthetic spectrum that matches the data (for more informa-  
 182 tion on this process, see below). The line lists were taken from  
 183 the CDMS (Müller et al. 2001; Müller et al. 2005) or the JPL  
 184 database (Pickett et al. 1998). Appendix A gives more informa-  
 185 tion on the spectroscopic studies used for our assignments and  
 186 Table B.2 presents the transitions covered in the data.

187 In the fitting process, the FWHM was first fitted for the  
 188 unblended line(s) of each molecule. Then it was fixed to that  
 189 value when the column density and excitation temperature were  
 190 being determined. The FWHM for all considered species is  
 191  $\sim 1.8 \pm 0.5 \text{ km s}^{-1}$ , except for (formic acid) t-HCOOH, which  
 192 is slightly lower (i.e.,  $\sim 1 \text{ km s}^{-1}$ ). The typical FWHM here is  
 193  $\sim 1.5 - 2$  times larger than the typical FWHM found in PILS  
 194 ( $\sim 1 \text{ km s}^{-1}$ ). However, the spectral resolution for the continuum  
 195 spectral window (i.e., the major spectral window where most  
 196 lines lie; Fig. B.1) is  $\sim 0.8 \text{ km s}^{-1}$  in this work. This implies  
 197 that not all lines are spectrally resolved. Therefore, the higher  
 198 FWHM measured here could be due to this low spectral reso-  
 199 lution. The excitation temperature was only fitted if there were  
 200 enough ( $\geq 2$ ) detected lines of a molecule with a range of  $E_{\text{up}}$   
 201 (e.g.,  $\sim 100 - 400 \text{ K}$ ). The typical uncertainty on the excitation  
 202 temperature is  $\sim \pm 50 \text{ K}$ . If not enough lines with a range of  
 203  $E_{\text{up}}$  were detected, the temperature is fixed to 100 K, which is  
 204 similar to excitation temperatures assumed or found for many

species in PILS (Lykke et al. 2017; Calcutt et al. 2018b; Jør-  
 205 gensen et al. 2018). The exceptions to this rule were t-HCOOH  
 206 and NH<sub>2</sub>CHO. Only one line was detected for each of these two  
 207 molecules and their temperatures were fixed to 300 K to be con-  
 208 sistent with PILS (Coutens et al. 2016; Jørgensen et al. 2018).  
 209 Moreover, for the isotopologues for which a determination of  
 210 the excitation temperature was not possible, the temperature was  
 211 fixed to that of the other isotopologues with a determined  $T_{\text{ex}}$ .  
 212 Deuterated methanol, CH<sub>2</sub>DOH, has three detected lines, with  
 213 upper energy levels of  $\sim 10 \text{ K}$ ,  $\sim 100 \text{ K}$ , and  $\sim 400 \text{ K}$ . It was not  
 214 possible to fit all three lines of this molecule with a single exci-  
 215 tation temperature. Therefore, we adopted the same temperature as  
 216 the methanol isotopologue that has the most lines detected (i.e.,  
 217 CHD<sub>2</sub>OH). However, this temperature fits the  $\sim 100 \text{ K}$  line bet-  
 218 ter than the other two. For aGg'-(CH<sub>2</sub>OH)<sub>2</sub>, we note that again a  
 219 single temperature cannot fit all of its lines. In particular, the line  
 220 at 90.593 GHz with  $E_{\text{up}} = 19 \text{ K}$  gets overestimated regardless of  
 221 the temperature assumed. This could be because of this line be-  
 222 ing (marginally) optically thick; therefore, we ignored this line  
 223 and fixed the temperature to that of gGg'-(CH<sub>2</sub>OH)<sub>2</sub>. A similar  
 224 two-component temperature structure was found for glycoloni-  
 225 trile (HOCH<sub>2</sub>CN) toward IRAS 16293 B (Zeng et al. 2019). Us-  
 226 ing this method the rest of the lines are explained reasonably  
 227 well (i.e., within  $\sim 20 - 30\%$ ; see Fig. B.1). 228

229 The column density was always treated as a free parame-  
 230 ter. The uncertainty on column densities was measured from the  
 231 same method explained in Nazari et al. (2022a) and the typi-  
 232 cal uncertainty from the fits is on the order of 20%. Figure B.1  
 233 shows the final fitted model for each molecule. As this figure  
 234 shows, there are still unidentified lines in the spectrum (see Sect.  
 235 3.1 for more details). In this process, the source velocity was  
 236 fixed to  $V_{\text{lsr}} = 2.7 \text{ km s}^{-1}$  and a beam dilution of unity was as-  
 237 sumed resulting in our column densities being representative of  
 238 those within a beam. This is different from the assumption in  
 239 PILS where the source size was set to  $0.5''$ . Nevertheless, this  
 240 assumption does not change the conclusions as long as the lines  
 241 are optically thin. This is because only the number of molecules  
 242 and their ratios are of interest here. The number of molecules  
 243 ( $N$ ) is constant regardless of the source size assumed. The num-  
 244 ber of molecules is equal to  $N \times A$ , where  $A$  is the emitting area.  
 245 Hence a decrease in the emitting area increases the fitted column  
 246 densities and vice versa such that the number of molecules stays  
 247 the same as long as the lines stay optically thin (also see van  
 248 Gelder et al. 2022a; Nazari et al. 2023c). However, we note that

<sup>1</sup> <http://cassis.irap.omp.eu/>



with this assumption, we ignored any potential differences between the emitting areas of various molecules. This assumption can only be improved with higher angular resolution data than presented in this work.

### 3. Results

#### 3.1. Deep search and the considered species

The spectrum of IRAS16293 B at  $\sim 3$  mm wavelengths is line rich and crowded (see Fig. 1 for an overview). In total, 16 molecules were detected and 15 were tentatively detected (see Table 1). Ratios of the detected molecules with respect to methanol are presented in the left panel of Fig. 2 (see Sect. 4.2.3 for a discussion on the comparison with PILS). Among these species, many "standard" COMs such as methanol ( $\text{CH}_3\text{OH}$ ), ethanol ( $\text{CH}_3\text{CH}_2\text{OH}$ ), ethyl cyanide ( $\text{CH}_3\text{CH}_2\text{CN}$ ), acetaldehyde ( $\text{CH}_3\text{CHO}$ ), methyl formate ( $\text{CH}_3\text{OCHO}$ ), and dimethyl ether ( $\text{CH}_3\text{OCH}_3$ ) with some of their isotopologues are apparent. The frequency range did not cover transitions of  $\text{CH}_3\text{CN}$  and  $\text{HNCO}$  or their isotopologues. We also detected one carbon chain molecule, cyanoacetylene ( $\text{HCCCN}$ ). It should be noted that the frequency range of the observations covers  $\text{HC}_5\text{N}$  transitions, but this carbon chain was not detected toward IRAS16293 B. It was, however, detected  $\sim 12''$  off-source to the west of IRAS16293 B (Murillo et al. 2022b).

This dataset was specifically taken to search for large species due to the expected lower line density and line confusion in Band 3 in comparison with Band 7 used for PILS. Moreover, at the same excitation temperature, heavier molecules have their Boltzmann distribution peak at lower frequencies, which increases the chance of detecting them in Band 3. Particularly, the frequency windows were selected to search for glycerol ( $\text{HOCH}_2\text{CH}(\text{OH})\text{CH}_2\text{OH}$ ) and propanol ( $\text{C}_3\text{H}_7\text{OH}$ ). Isopropanol (*i*- $\text{C}_3\text{H}_7\text{OH}$ ) and normal-propanol (*n*- $\text{C}_3\text{H}_7\text{OH}$ ) have been detected previously in the ISM (Belloche et al. 2022; Jiménez-Serra et al. 2022), although not yet in IRAS16293 B (Taquet et al. 2018). In addition to these molecules, we searched for and detected large and complex species such as aGg'- and gGg'-ethylene glycol ( $(\text{CH}_2\text{OH})_2$ ), glycolaldehyde ( $\text{CH}_2\text{OHCHO}$ ), and acetone ( $\text{CH}_3\text{COCH}_3$ ).

Table B.1 presents the upper limits of the molecules we searched for but do not detect, including glycerol and isopropanol. The largest molecule that we searched for is cyanonaphthalene ( $\text{C}_{10}\text{H}_7\text{CN}$ ; McNaughton et al. 2018) and its upper limit is given in Table B.1. Figures 3, B.2, and B.3 present the lines of *g*-Isopropanol, *Ga*-*n*-propanol, and *G'Gg'gg'*-Glycerol with the model upper limits. We note that in Fig. 3, the lines that seem to agree well with the data in the first two panels are well explained with other molecules (see the cyan line as the total fitted model for the detected or tentatively detected species), and thus they could not be the lines of *g*-Isopropanol. Moreover, the line at around 91.345 GHz overestimates the data. The ratio of measured upper limits with respect to methanol are presented in the right panel of Fig. 2. The ratios span a range of  $\sim 5$  orders of magnitude from  $\sim 10^{-6}$  to  $\sim 0.1$ , which is similar to the range seen for the detected molecules (left panel of Fig. 2).

The line density of the lines detected at  $\geq 6\sigma$  level in Band 3 ( $\sim 100$  GHz) data is one per  $\sim 8.5$  MHz (see Fig. B.1 for the variations in line density across the frequency range), while the line density is one per  $\sim 3.5$  MHz in Band 7 ( $\sim 345$  GHz; Jørgensen et al. 2016). Therefore, as expected, the spectrum has a lower line density in Band 3 than Band 7, although only by a factor of  $\sim 2.5$ , resulting in a relatively line-rich spectrum still. Although

Table 1: Fitted parameters for detected and tentatively detected Band 3 species toward IRAS 16293 B.

| Species   | $N$<br>( $\text{cm}^{-2}$ )        | $T_{\text{ex}}$<br>(K) | $N_{\text{X}}/N_{\text{CH}_3\text{OH}}$ | # Detected lines |
|---|------------------------------------|------------------------|---|------------------|
| $^{13}\text{CH}_3\text{OH}$                     | $1.2^{+0.4}_{-0.2} \times 10^{17}$ | $130^{+30}_{-20}$      | $1.5^{+0.7}_{-0.4} \times 10^{-2}$      | 2                |
| $\text{CH}_2\text{DOH}$                         | $1.5^{+0.1}_{-0.3} \times 10^{17}$ | [170]                  | $1.8^{+0.6}_{-0.5} \times 10^{-2}$      | 3                |
| $\text{CHD}_2\text{OH}$                         | $1.9^{+0.4}_{-0.3} \times 10^{17}$ | $170^{+40}_{-40}$      | $2.3^{+0.9}_{-0.6} \times 10^{-2}$      | 9                |
| $\text{CD}_3\text{OH}$                          | $5.6^{+0.7}_{-0.9} \times 10^{16}$ | [170]                  | $6.9^{+2.4}_{-1.8} \times 10^{-3}$      | 1                |
| $\text{CH}_3\text{CHO}$                         | $3.5^{+0.2}_{-0.4} \times 10^{16}$ | $70^{+20}_{-10}$       | $4.3^{+1.5}_{-1.0} \times 10^{-3}$      | 3                |
| $^{13}\text{CH}_3\text{CHO}$                    | $2.1^{+0.3}_{-0.3} \times 10^{15}$ | [100]                  | $2.6^{+0.9}_{-0.7} \times 10^{-4}$      | 2                |
| $\text{CH}_2\text{DCHO}$                        | $4.0^{+0.5}_{-0.5} \times 10^{15}$ | [100]                  | $4.9^{+1.7}_{-1.2} \times 10^{-4}$      | 2                |
| $\text{CH}_3\text{CDO}$                         | $5.0^{+2.0}_{-2.0} \times 10^{15}$ | $110^{+30}_{-30}$      | $6.1^{+3.2}_{-2.8} \times 10^{-4}$      | 3                |
| $\text{CHD}_2\text{CHO}$                        | $3.0^{+0.5}_{-0.8} \times 10^{15}$ | [100]                  | $3.7^{+1.4}_{-1.2} \times 10^{-4}$      | 3                |
| $\text{CH}_3\text{COOH}$                        | $1.0^{+0.6}_{-0.2} \times 10^{16}$ | $170^{+30}_{-70}$      | $1.2^{+0.8}_{-0.4} \times 10^{-3}$      | 3                |
| $\text{CH}_2\text{OHCHO}$                       | $4.6^{+0.6}_{-0.6} \times 10^{16}$ | $280^{+20}_{-40}$      | $5.6^{+2.0}_{-1.4} \times 10^{-3}$      | 6                |
| $^{13}\text{CH}_2\text{OHCHO}$                  | $\sim 2.0 \times 10^{15}$          | [280]                  | $\sim 2.4 \times 10^{-4}$               | 2                |
| $\text{CHDOHCHO}$                               | $2.5^{+0.8}_{-0.8} \times 10^{15}$ | $120^{+50}_{-50}$      | $3.1^{+1.5}_{-1.2} \times 10^{-4}$      | 4                |
| $\text{CH}_3\text{CH}_2\text{OH}$               | $6.2^{+0.8}_{-0.7} \times 10^{16}$ | $170^{+20}_{-20}$      | $7.7^{+2.7}_{-1.8} \times 10^{-3}$      | 5                |
| <i>a-a</i> - $\text{CH}_2\text{DCH}_2\text{OH}$ | $2.4^{+0.5}_{-0.3} \times 10^{16}$ | [170]                  | $3.0^{+1.1}_{-0.7} \times 10^{-3}$      | 1                |
| <i>a-CH}_3\text{CHDOH}</i>                      | $2.1^{+0.4}_{-0.3} \times 10^{16}$ | [170]                  | $2.5^{+1.0}_{-0.6} \times 10^{-3}$      | 3                |
| $\text{CH}_3\text{OCHO}$                        | $8.5^{+2.5}_{-2.5} \times 10^{16}$ | $100^{+20}_{-20}$      | $1.0^{+0.4}_{-0.4} \times 10^{-2}$      | 10               |
| $\text{CH}_3\text{OCH}_3$                       | $1.0^{+0.1}_{-0.2} \times 10^{17}$ | $140^{+20}_{-30}$      | $1.2^{+0.4}_{-0.4} \times 10^{-2}$      | 10               |
| <i>aGg'</i> -( $\text{CH}_2\text{OH}$ ) $_2$    | $\sim 1.4 \times 10^{17}$          | [160]                  | $\sim 1.7 \times 10^{-2}$               | 15               |
| <i>gGg'</i> -( $\text{CH}_2\text{OH}$ ) $_2$    | $5.0^{+1.7}_{-1.4} \times 10^{16}$ | $160^{+40}_{-40}$      | $6.1^{+2.9}_{-2.1} \times 10^{-3}$      | 15               |
| $\text{D}_2\text{CO}$                           | $6.9^{+0.6}_{-0.6} \times 10^{15}$ | [100]                  | $8.5^{+2.9}_{-1.9} \times 10^{-4}$      | 1                |
| HCCCN   | $6.2^{+0.9}_{-0.8} \times 10^{13}$ | [100]                  | $7.6^{+2.8}_{-1.8} \times 10^{-6}$      | 1                |
| $\text{CH}_3\text{CH}_2\text{CN}$               | $1.4^{+0.2}_{-0.1} \times 10^{16}$ | [100]                  | $1.8^{+0.7}_{-0.4} \times 10^{-3}$      | 1                |
| $\text{NH}_2\text{CHO}$                         | $5.6^{+1.2}_{-1.1} \times 10^{16}$ | [300]                  | $6.8^{+2.7}_{-1.9} \times 10^{-3}$      | 1                |
| $\text{CH}_3\text{COCH}_3$                      | $1.6^{+0.6}_{-0.5} \times 10^{16}$ | $130^{+20}_{-20}$      | $2.0^{+1.0}_{-0.7} \times 10^{-3}$      | 17               |
| <i>t</i> -HCOOH                                 | $7.7^{+1.1}_{-1.1} \times 10^{16}$ | [300]                  | $9.5^{+3.4}_{-2.4} \times 10^{-3}$      | 1                |
| <i>c-C}_2\text{H}_4\text{O}</i>                 | $5.5^{+0.7}_{-0.5} \times 10^{15}$ | [100]                  | $6.7^{+2.4}_{-1.5} \times 10^{-4}$      | 2                |
| <i>c-C}_2\text{H}_3\text{DO}</i>                | $1.2^{+0.2}_{-0.2} \times 10^{15}$ | [100]                  | $1.5^{+0.5}_{-0.4} \times 10^{-4}$      | 2                |
| $\text{CH}_3\text{SH}$                          | $4.5^{+0.5}_{-0.7} \times 10^{15}$ | [100]                  | $5.5^{+1.9}_{-1.4} \times 10^{-4}$      | 2                |
| $\text{HOCH}_2\text{CN}$                        | $1.0^{+0.1}_{-0.1} \times 10^{15}$ | [100]                  | $1.2^{+0.4}_{-0.3} \times 10^{-4}$      | 2                |

**Notes.** Measured column densities toward the  $0.5''$  offset position from B in a  $\sim 1''$  beam. If a source size of  $0.5''$  was assumed, these column densities would increase by a factor of five (i.e.,  $\frac{0.5^2+1^2}{0.5^2}$ ). The major isotopologue of methanol was detected, but its column density was calculated by scaling the  $^{13}\text{CH}_3\text{OH}$  column density by  $^{12}\text{C}/^{13}\text{C} = 68$  (Milam et al. 2005). The FWHM for all molecules is  $\sim 1.8 \pm 0.5 \text{ km s}^{-1}$ . Species whose excitation temperature is fixed have their temperature given in square brackets. The right-most column gives an estimate of the number of relatively unblended lines that were detected for each molecule. Those detected with only one line should be taken with caution. However, we note that all of these species are detected in PILS (see the text for references).

many lines ( $\sim 70\%$ ) in the Band 3 spectrum of IRAS16293 B were identified, we could not associate any simple or complex species to  $\sim 25 - 30\%$  of lines at the  $\geq 6\sigma$  level. Potentially more high-resolution laboratory spectra are needed to identify those lines. This is particularly important for the (doubly) deuterated isotopologues of known COMs and larger COMs with more than eight atoms.

#### 3.2. Fitting results for the detected species

Derived column densities and excitation temperatures are given in Table 1. The measured excitation temperatures span a range

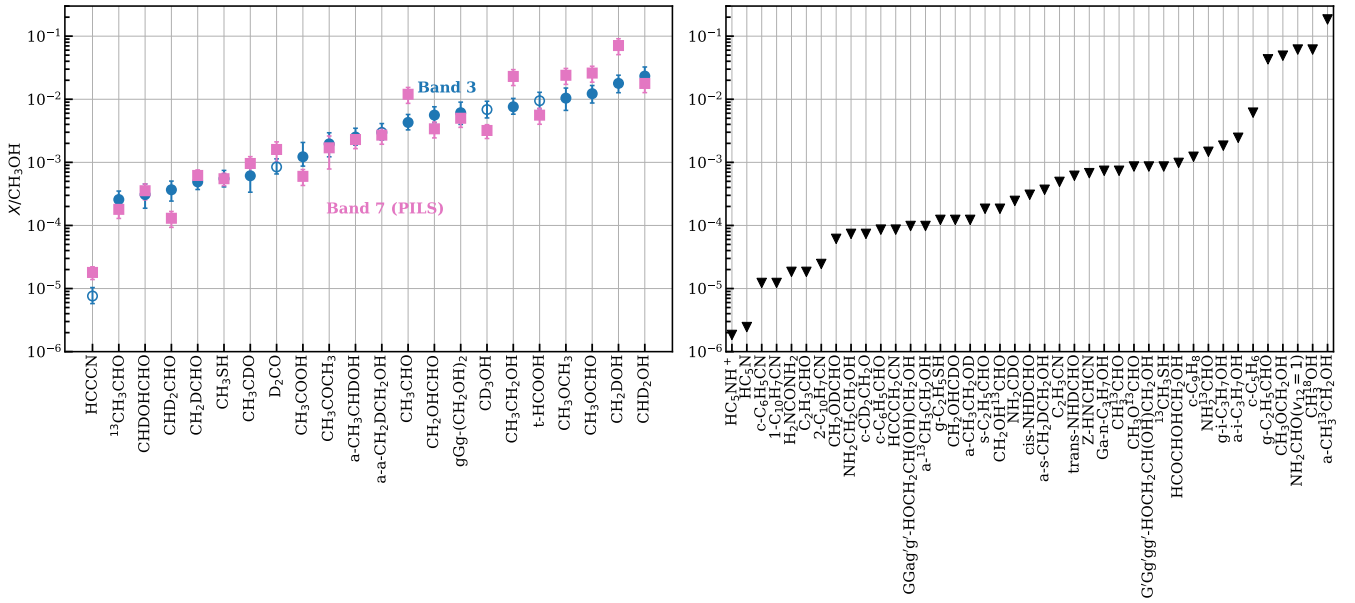


Fig. 2: Column density ratios of detected species and upper limits with respect to methanol. Left: Column density ratios for the detected species with respect to methanol for our Band 3 data (blue). The same ratios from PILS in Band 7 (pink) are also shown for comparison (see the text for references). The hollow symbols show the species that only have one detected line. Right: Ratios of the upper limits measured in this work (Table B.1) with respect to methanol. In both panels, the species are ordered from left to right by increasing Band 3 ratios with respect to methanol.

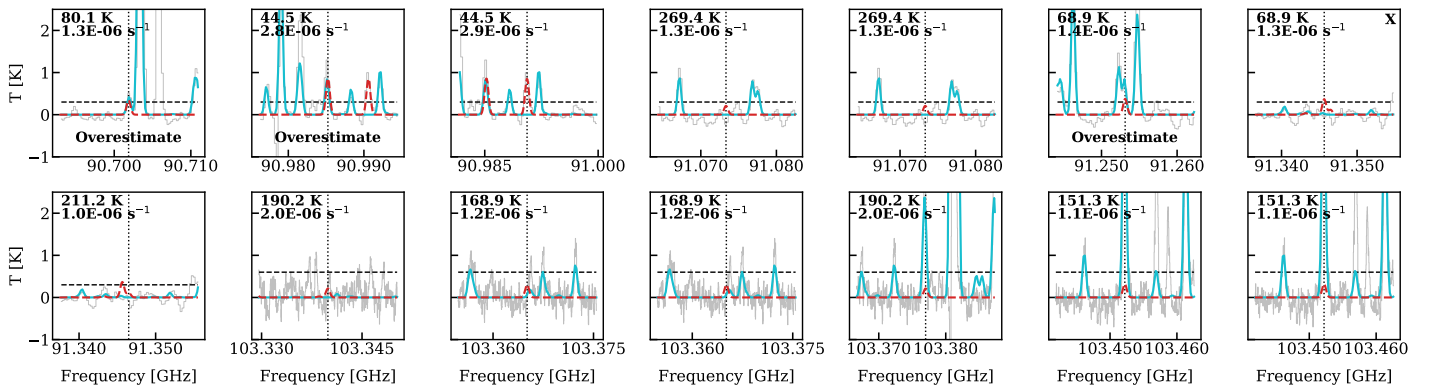


Fig. 3: Lines of g-Isopropanol and the model for its upper limit in red dashed lines ( $1.5 \times 10^{16} \text{ cm}^{-2}$ ). Gray is the data and cyan is the total fitted model from the detected and tentatively detected species. The vertical dotted lines show the transition frequency of each line. The  $E_{\text{up}}$  and  $A_{ij}$  are printed in the top left of each panel. The line that was used to find the  $3\sigma$  upper limit is indicated by an "X" in the top right. The horizontal dashed lines show the  $3\sigma$  level. Only lines with  $A_{ij} > 10^{-6} \text{ s}^{-1}$  and  $E_{\text{up}} < 300 \text{ K}$  are shown.

between  $\sim 50$  and  $\sim 300 \text{ K}$ . Figure B.4 presents the excitation temperatures where a determination was possible for molecules with sufficient detected lines. The species on the x-axis are roughly ordered by increasing binding energies in the ice from left to right (Minissale et al. 2022; Ligterink & Minissale 2023). The error bars are too large to robustly confirm whether there is any correlation between the excitation temperature and binding energy.

The column densities measured here span a range of  $\sim 4$  orders of magnitude. The most abundant molecule is methanol, after that (and its isotopologues),  $\text{CH}_3\text{OCHO}$  and  $\text{CH}_3\text{OCH}_3$  were found to be the second and third most abundant species as found in many other protostellar systems (Coletta et al. 2020; Chen et al. 2023). The column density of  $\text{CH}_3\text{OH}$  was determined by scaling the  $^{13}\text{C}/^{12}\text{C}$  column density by  $^{12}\text{C}/^{13}\text{C}$  of 68 (Milam

et al. 2005) and was found to be  $8.2 \times 10^{18} \text{ cm}^{-2}$  in the  $\sim 1''$  beam. We note that the  $^{13}\text{CH}_3\text{OH}$  lines used for measurement of column density of this molecule are relatively weak and hence optically thin. They either have a large  $E_{\text{up}}$  ( $\sim 500 \text{ K}$ ) or a low  $A_{ij}$  ( $\sim 6 \times 10^{-8} \text{ s}^{-1}$ ). Therefore,  $^{13}\text{CH}_3\text{OH}$  in this study should robustly determine the column density of the major isotopologue without the need for  $\text{CH}_3^{18}\text{OH}$ . The least abundant molecule at the  $0.5''$  offset location is HCCCN with a column density of  $6.2 \times 10^{13} \text{ cm}^{-2}$  (see Murillo et al. 2022b for its map).

### 3.3. Glycolonitrile and ethylene oxide

Here we focus on the tentative detection of  $\text{HOCH}_2\text{CN}$  (glycolonitrile) and  $\text{c-C}_2\text{H}_4\text{O}$  (ethylene oxide). These two molecules

are among the less common species studied toward protostars in Table 1. Glycolonitrile is an interesting interstellar molecule to study given that it is a rarely observed prebiotic molecule. Ethylene oxide is an interesting molecule because it is the only species in Table 1 with a cyclic structure.

Glycolonitrile was detected toward IRAS 16293 B using lower frequency ( $\lesssim 266$  GHz) observations than PILS (Zeng et al. 2019). Later it was also detected in PILS by Ligterink et al. (2021), mainly toward the half-beam offset position ( $\sim 0.25''$  offset from the continuum peak) and not the full-beam offset position ( $0.5''$  offset). It is interesting that in the Band 3 data, HOCH<sub>2</sub>CN was tentatively detected toward the full-beam offset position of PILS. This could be due to the larger beam size of the Band 3 observations and the inclusion of the hotter gas close to the protostar in the beam given that the binding energy of this molecule is relatively high ( $\sim 10$  400 K; Ligterink & Minissale 2023).

Our tentative column density ratio of HOCH<sub>2</sub>CN/CH<sub>3</sub>OH ( $\sim 10^{-4}$ ) agrees well with what Ligterink et al. (2021) found for this source in Band 7. Moreover, our column density for HOCH<sub>2</sub>CN, after correction for beam dilution (see Sect. 4.2.2), is within a factor of about two of what Zeng et al. (2019) found for their warm component of the same source from their Band 3 data. Moreover, glycolonitrile has been (tentatively) detected toward other objects such as the Serpens SMM1-a protostar and the G+0.693-0.027 molecular cloud with similar HOCH<sub>2</sub>CN/CH<sub>3</sub>OH ratios of a few  $10^{-4}$  (Requena-Torres et al. 2006; Ligterink et al. 2021; Rivilla et al. 2022). A recent study searched for its minor isotopologues in IRAS16293B and SMM1-a, but it resulted in non-detections (Margulès et al. 2023).

Ethylene oxide has been detected toward several objects, mainly high-mass protostars, but also pre-stellar cores and the comet 67P (Dickens et al. 1997; Nummelin et al. 1998; Ikeda et al. 2001; Requena-Torres et al. 2008; Bacmann et al. 2019; Drozdovskaya et al. 2019). This molecule has also been detected toward IRAS16293 A and B by PILS (Lykke et al. 2017; Manigand et al. 2020). The ratio for ethylene oxide to methanol from this work is  $\sim 7 \times 10^{-4}$ , which agrees well with the ratio from PILS of  $\sim 3 - 6 \times 10^{-4}$  (Lykke et al. 2017; Jørgensen et al. 2016, 2018). Its deuterated species were studied and detected toward IRAS16293 B by Müller et al. (2023a,b). We also tentatively detected one of its deuterated species, c-C<sub>2</sub>H<sub>3</sub>DO, in our Band 3 data. The ratio of this molecule with respect to methanol in our data is  $\sim 1 - 2 \times 10^{-4}$  which agrees well with the same ratio in PILS ( $\sim 9 \times 10^{-5}$ ; Jørgensen et al. 2018; Müller et al. 2023a).

## 4. Discussion

### 4.1. Dust optical depth

For this section we calculated the continuum optical depth at  $\sim 348.815$  GHz (corresponding to ALMA Band 7) and at  $\sim 91$  GHz (corresponding to ALMA Band 3). The continuum optical depth as a zeroth-order approximation is given by (see Rivilla et al. 2017 and van Gelder et al. 2022b)

$$\tau_\nu = -\ln\left(1 - \frac{F_\nu}{\Omega_{\text{beam}} B_\nu(T_{\text{dust}})}\right), \quad (1)$$

where  $F_\nu$  is the continuum flux density within the beam,  $\Omega_{\text{beam}} = \pi\theta_{\text{min}}\theta_{\text{maj}}/(4 \ln(2))$  is the beam solid angle with  $\theta_{\text{min}}$  and  $\theta_{\text{maj}}$  as the beam minor and major axes,  $B_\nu$  is the Planck function, and  $T_{\text{dust}}$  is the dust temperature. We took the continuum image of the PILS survey at  $\nu \sim 348.815$  GHz from the ALMA archive and

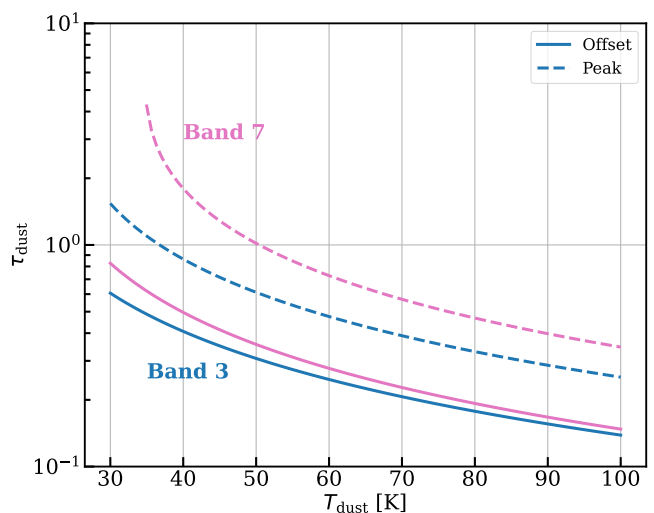


Fig. 4: Continuum optical depth as a function of temperature at the peak of the continuum (dashed) and the  $0.5''$  offset position where the spectrum was extracted (solid line). Blue shows the optical depth for the Band 3 continuum at a frequency of  $\sim 91$  GHz and pink shows the PILS continuum at a frequency of  $\sim 348.815$  GHz.

found  $F_\nu$  to be within the beam of those observations at the peak of the continuum and at the  $\sim 0.5''$  offset position where the spectrum was extracted. For this measurement we used CASA (McMullin et al. 2007) version 6.5.2.26 and found the continuum flux density to be  $\sim 1.16 \text{ Jy beam}^{-1}$  and  $\sim 0.55 \text{ Jy beam}^{-1}$  at the peak and the offset position. We did the same for the Band 3 data at a frequency of  $\sim 91$  GHz and found the Band 3 continuum flux density to be  $\sim 9.07 \times 10^{-2} \text{ Jy beam}^{-1}$  and  $\sim 5.25 \times 10^{-2} \text{ Jy beam}^{-1}$  at the peak and the offset positions, respectively. Next, we calculated  $\tau_{\text{dust}}$  for a range of dust temperatures that are feasible for IRAS16293B as suggested by Jacobsen et al. (2018).

Figure 4 presents the continuum optical depth for the various temperatures. The temperature of the inner regions based on models of Jacobsen et al. (2018) is  $\sim 90$  K. At 90 K, both the PILS and Band 3 peak continuum are marginally optically thick with the PILS continuum having an optical depth of  $\sim 1.5$  times larger. However, at the location off-source, the dust optical depth for the PILS continuum is almost the same as that of Band 3, which is  $\sim 0.15$ . Therefore, it is safe to assume that the dust at the offset location at  $T_{\text{dust}} = 90$  K is almost completely optically thin in Band 3 and Band 7 datasets. Even assuming the unrealistic worst case scenario of  $T_{\text{dust}} = 30$  K in Fig. 4 and assuming that all the dust is in a column between the observer and the protostar, the difference between Band 3 and Band 7 dust attenuation (i.e.,  $e^{-\tau}$ ) is around 25% at the offset location at most.

### 4.2. Comparison with PILS

In this section we compare the excitation temperatures and column densities of the same molecules detected in the PILS Band 7 survey and this work.

#### 4.2.1. Excitation temperature

The measured excitation temperatures are presented in Fig. B.4. The species are roughly ordered by increasing binding energy (a



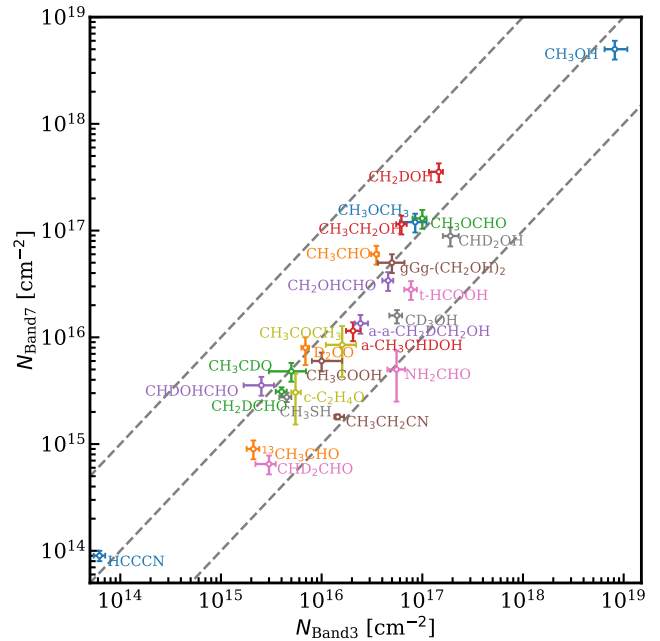
436 measure of how strongly bound a molecule is in ices) from left to  
 437 right. However, given that the uncertainties are relatively large,  
 438 the number of detected lines for each species is small, and the  
 439 lines are biased toward lower  $E_{\text{up}}$ ; it is not possible to identify  
 440 a clear trend between the binding energies (or sublimation tem-  
 441 peratures) and excitation temperatures. Another effect that can  
 442 complicate the picture and change Fig. B.4 is that the molecules  
 443 with lower binding energies than water are expected to desorb  
 444 with water if initially mixed with it (Collings et al. 2004; Busch  
 445 et al. 2022; Garrod et al. 2022). This would be in line with the  
 446 measured excitation temperatures of the molecules toward the  
 447 left hand side of Fig. B.4 being at around  $\sim 100$  K (i.e., the des-  
 448 orption temperature of water). Therefore, a strong trend might  
 449 not be expected in Fig. B.4.

450 Nevertheless, our excitation temperatures mostly agree with  
 451 those found by Jørgensen et al. (2018) for IRAS16293 B. The  
 452 only exceptions are  $\text{CH}_3\text{OCHO}$  and  $\text{CH}_3\text{CH}_2\text{OH}$  where their ex-  
 453 citation temperatures are found to be higher in PILS. This could  
 454 be due to the lines that are covered in the Band 3 data having a  
 455 lower  $E_{\text{up}}$  than those covered in the Band 7 data. For example,  
 456 if the two lines of  $\text{CH}_3\text{CH}_2\text{OH}$  with  $E_{\text{up}} \sim 80 - 90$  K are ignored,  
 457 a fit at  $T_{\text{ex}} \sim 240$  K (i.e., agreeing with the PILS temperature) can  
 458 match the brightness temperatures of the rest of the lines within  
 459  $\sim 40 - 50\%$ . Our excitation temperatures also agree well with  
 460 what is found for the companion source, IRAS16293A, in PILS  
 461 (Manigand et al. 2020).

#### 462 4.2.2. Column density

463 Making a direct comparison of the column densities from PILS  
 464 and this work should be done with caution due to the differ-  
 465 ent beam sizes in the two sets of observations. Therefore, be-  
 466 fore comparison, column densities of Band 7 were corrected to  
 467 match the Band 3 results. PILS studies use a source size of  $0.5''$   
 468 in their analysis, while we found the column densities averaged  
 469 over the Band 3 beam. Our assumption corresponds to the Band  
 470 3 emission filling the beam uniformly (i.e.,  $\theta_s \gg \theta_b$ ). The PILS  
 471 column densities were converted to an average over the PILS  
 472 beam (or filling the PILS beam uniformly) by multiplication with  
 473 their beam dilution factor of  $\frac{0.5^2}{0.5^2+0.5^2} = 0.5$ . After this modifica-  
 474 tion, we also investigated how the different beam sizes in PILS  
 475 and our study can affect the comparison (assuming that the col-  
 476 umn densities are averaged over the respective beams). Figure  
 477 B.5 presents a two-dimensional Gaussian distribution with two  
 478 circular regions representing the beams of Band 3 and Band 7.  
 479 Assuming a uniform beam, we calculated the mean in the two  
 480 beams and found around a 10% difference between these two,  
 481 which is smaller than the typical uncertainties on the column  
 482 densities and it was thus ignored.

483 Figure 5 presents the column densities from PILS and this  
 484 work after correction for beam dilution. The column densities of  
 485 PILS are taken from Coutens et al. (2016) ( $\text{NH}_2\text{CHO}$ ), Jørgensen  
 486 et al. (2016) ( $\text{CH}_2\text{OHCHO}$ ,  $\text{CHDOHCHO}$ ,  $\text{gGg}-(\text{CH}_2\text{OH})_2$ ,  
 487 and  $\text{CH}_3\text{COOH}$ ), Calcutt et al. (2018b) ( $\text{CH}_3\text{CH}_2\text{CN}$ ,  $\text{HC}_3\text{N}$ ),  
 488 Jørgensen et al. (2018) ( $\text{CH}_3\text{OH}$ ,  $^{13}\text{CH}_3\text{CHO}$ ,  $\text{CH}_3\text{CDO}$ ,  
 489  $\text{CH}_3\text{CHO}$ ,  $\text{CH}_2\text{DOH}$ ,  $\text{CH}_3\text{CH}_2\text{OH}$ ,  $\alpha\text{-CH}_3\text{CHDOH}$ ,  $\text{CH}_3\text{OCH}_3$ ,  
 490  $\text{CH}_3\text{OCHO}$ ,  $\alpha\text{-a-CH}_2\text{DCH}_2\text{OH}$ , and  $\text{t-HCOOH}$ ), Persson et al.  
 491 (2018) ( $\text{D}_2\text{CO}$ ), Manigand et al. (2020) ( $\text{CH}_2\text{DCHO}$ ), Droz-  
 492 dovskaya et al. (2022) ( $\text{CHD}_2\text{OH}$ ), Ilyushin et al. (2022)  
 493 ( $\text{CD}_3\text{OH}$ ), Drozdovskaya et al. (2018) ( $\text{CH}_3\text{SH}$ ), Ferrer Asen-  
 494 sio et al. (2023) ( $\text{CHD}_2\text{CHO}$ ), and Lykke et al. (2017)  
 495 ( $\text{CH}_3\text{COCH}_3$ ). In addition, we did not include  $^{13}\text{CH}_2\text{OHCHO}$   
 496 and  $\text{gGg}-(\text{CH}_2\text{OH})_2$  in Fig. 5 because our measured column



497 Fig. 5: Column density of the various molecules from the ALMA  
 498 Band 7 observations (PILS;  $\sim 345$  GHz) as a function of those  
 499 from Band 3 ( $\sim 100$  GHz). Beam dilution was corrected for the  
 500 column densities in this figure. Dashed lines present where the  
 501 values of the y-axis are the same as the values of the x-axis,  
 502 where they are ten times higher and ten times lower than the  
 503 values of the x-axis.

497 densities are approximate. Moreover, the column density of  
 498  $\text{CH}_3\text{COOH}$  in PILS was found from old spectroscopic data  
 499 (Jørgensen et al. 2016). To avoid a bias, we redid the fit to  
 500  $\text{CH}_3\text{COOH}$  in the Band 7 data using new spectroscopic data  
 501 (Ilyushin et al. 2013; see Appendix A), and found that the col-  
 502 umn density in Jørgensen et al. (2016) was underestimated by a  
 503 factor of about two. Therefore, in this work we refer to the up-  
 504 dated column density of  $\text{CH}_3\text{COOH}$  using the new spectroscopic  
 505 data ( $\sim 1.2 \times 10^{16}$ ).

506 Figure 5 shows that the column densities from the Band  
 507 3 observations generally agree with those of PILS. There are  
 508 a few data points where the Band 3 column densities are  $\geq 3$   
 509 times higher than those of Band 7. Among those molecules,  
 510  $\text{NH}_2\text{CHO}$  and  $\text{CH}_3\text{CH}_2\text{CN}$  seem to be outliers that have Band  
 511 3 column densities that are ten times higher than Band 7. How-  
 512 ever, because the column densities of these two molecules in this  
 513 work were measured based on only one line, those values should  
 514 be considered with caution. Therefore, we excluded these two  
 515 molecules from further analysis.

516 Taking only the molecules with at least three detected lines  
 517 in Band 3 (see Table 1), the average of ( $\log_{10}$  of) the Band 3 col-  
 518 umn densities weighted by the uncertainty on each data point is  
 519  $4.4 \times 10^{16} \text{ cm}^{-2}$ . This value for Band 7 column densities (mea-  
 520 sured using many more lines per molecule due to the larger  
 521 frequency coverage) is  $2.7 \times 10^{16} \text{ cm}^{-2}$ . These two agree well  
 522 within the uncertainties. Moreover, the scatter around the line of  
 523  $N_{\text{Band3}} = N_{\text{Band7}}$  is a factor of 1.9 below the line and 1.8 above the  
 524 line. Therefore, it can be concluded that there is a tight, one-to-  
 525 one correlation between the two column densities with a scatter  
 526 of less than a factor of two. This agrees well with the low dust

527 optical depth found for the Band 3 and Band 7 observations at  
528 the offset location where the spectra were extracted.

#### 529 4.2.3. Ratios

530 The column density ratios are normally more informative than  
531 absolute column densities because the latter depends on the  
532 beam and the assumed beam dilution factor. The left panel of  
533 Fig. 2 shows that the ratios with respect to methanol from Band  
534 3 agree well with those from Band 7 (PILS) for almost all  
535 molecules. Figure 6 presents the ratio between the Band 3 and  
536 Band 7 results for individual molecules. This figure shows, even  
537 more clearly, that the results from the Band 3 data (this work)  
538 generally agree within a factor of about two with the results from  
539 the Band 7 data. Four molecules show larger than a factor of two  
540 difference between the two datasets and they are marked with an  
541 ellipse. This could be due to the lines of these species becoming  
542 optically thick. This argument is more convincing for  $\text{CH}_3\text{CHO}$   
543 and  $\text{CH}_3\text{CH}_2\text{OH}$  given that there is good agreement between  
544 Band 3 and Band 7 results for their minor isotopologues. More-  
545 over, the value for  $\text{CH}_2\text{DOH}$  is likely uncertain given that no  
546 single temperature could be fitted to its lines and hence the as-  
547 sumed  $T_{\text{ex}}$  does not fit all its lines equally well in this work (see  
548 Sect. 2.2). The slight variations between the Band 3 and Band 7  
549 ratios could be due to the smaller number of lines covered in the  
550 Band 3 dataset compared with the PILS dataset, which also sets  
551 looser constraints on the excitation temperatures. Another factor  
552 in these variations could be the different beam sizes in the two  
553 datasets (see Sect. 4.2.2).

554 We found a good match between Band 3 and Band 7 data  
555 when comparing the ratios of the various COMs relative to  
556 methanol. The molecules that have column densities with a factor  
557 of  $> 2$  difference between Band 3 and Band 7 in Fig. 5 (i.e.,  
558  $t\text{-HCOOH}$ ,  $\text{CD}_3\text{OH}$ , and  $\text{CHD}_2\text{CHO}$ ) show good agreement (factor  
559 of  $< 2$ ) when their column density ratios with respect to  
560 methanol are compared between the two sets of observations.

#### 561 4.3. Comparison with other studies

562 In this section we put some of the measured ratios (Fig. 2) in the  
563 context of other works. We mainly focus on the upper limit ratios  
564 because similar comparisons have been made in the PILS papers  
565 between the measured column density ratios of IRAS 16293  
566 B and other sources. The ratios of  $a\text{Gg}'$ - and  $g\text{Gg}'$ - $(\text{CH}_2\text{OH})_2$   
567 to  $\text{CH}_3\text{OH}$  from our observations is between  $\sim 4 \times 10^{-3}$  and  
568  $\sim 2 \times 10^{-2}$ . The laboratory experiments and Monte Carlo simu-  
569 lations found the  $(\text{CH}_2\text{OH})_2/\text{CH}_3\text{OH}$  ratio to be  $\sim 10^{-2} - 9 \times 10^{-2}$   
570 and  $\sim 2 \times 10^{-2} - 4 \times 10^{-2}$  (Fedoseev et al. 2015), which agrees with  
571 our observations. Moreover, Fedoseev et al. (2017) found a ratio  
572 of glycerol/ethylene glycol upper limit of around 0.01 in labora-  
573 tory experiments which, from the ethylene glycol/methanol ratio  
574 of Fedoseev et al. (2015), gives a glycerol/methanol upper limit  
575 of between  $10^{-4}$  and  $9 \times 10^{-4}$ . Our upper limit ratios of  $\text{GGag}'g'$ -  
576 and  $\text{G}'\text{Gg}'\text{gg}'$ -glycerol to methanol are  $< 10^{-4}$  and  $< 8 \times 10^{-4}$ ,  
577 which are on the same order of magnitude as reported in labora-  
578 tory experiments and Monte Carlo simulations (Fedoseev et al.  
579 2015, 2017).

580 Propanal was found to form n-propanol (Qasim et al.  
581 2019a,b), and both were not detected in the Band 3 data. How-  
582 ever, we note that propanal was detected toward IRAS 16293 B  
583 by PILS (Lykke et al. 2017) and Qasim et al. (2019a) found that  
584 the ratio of their upper limit ratio for n-propanol/propanal for  
585 IRAS 16293 B is consistent with their laboratory experiments.

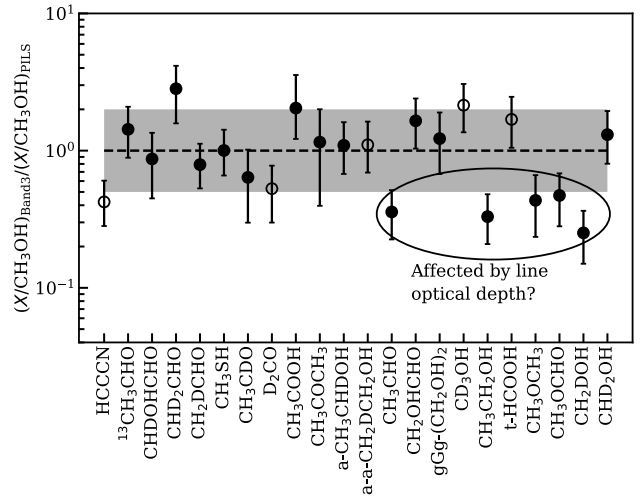


Fig. 6: Ratio between Band 3 and PILS column density ratios with respect to methanol (i.e., the ratio of blue to pink from the left panel of Fig. 2). The horizontal dashed line indicates where the ratio between Band 3 and PILS are the same. The shaded gray area indicates the region with a factor of two difference between Band 3 and PILS results. The species are ordered in the same way as in the left panel of Fig. 2. The hollow symbols show the species that have only one detected line.

Our upper limit ratio of Ga-n-propanol/methanol is  $< 7 \times 10^{-4}$ , which is a factor of about six lower than the detected ratio toward G+0.693-0.027 ( $\sim 4 \times 10^{-3}$ ; Jiménez-Serra et al. 2022 and Rodríguez-Almeida et al. 2021). Our upper limit ratios of g-, a-Isopropanol, and Ga-n-propanol with respect to methanol agree within a factor of about two with those detected toward Sgr B2(N2b) ( $\sim 0.002$ ; Belloche et al. 2022). Band 3 ratios of s- and g-propanal/methanol are  $< 2 \times 10^{-4}$  and  $< 0.04$ , respectively. These are in agreement with the abundance ratios of propanal/methanol in TMC-1 (around 0.01, Agúndez et al. 2023) and PILS (around  $2 \times 10^{-4}$ ; Lykke et al. 2017). Moreover, the abundance of indene with respect to  $\text{H}_2$  toward TMC-1 (Cernicharo et al. 2021) is on the same order of magnitude as our upper limit ratio of indene/ $\text{H}_2$ , assuming a lower limit on the  $\text{H}_2$  column density of  $10^{25} \text{ cm}^{-2}$  from Jørgensen et al. (2016) for IRAS 16293 B. However, using the same lower limit column density for  $\text{H}_2$  toward IRAS 16293 B, our upper limit abundances of 1-CNN, 2-CNN, and benzonitrile are a factor of about two to ten lower than what is found for TMC-1 (Gratier et al. 2016; McGuire et al. 2021).

The Band 3 upper limit ratio of urea/methanol is  $< 2 \times 10^{-5}$ , which is in-line and on the lower end of the observed range (either upper limit or detected) in the literature toward SgrB2 (Belloche et al. 2019), NGC 6334I (Ligterink et al. 2020), and G+0.693-0.027 systems (Zeng et al. 2023). The upper limit  $\text{NH}^{13}\text{CHO}/\text{CH}_3\text{OH}$  in this work is consistent with the detected ratios toward NGC 6334I (Ligterink et al. 2020; methanol from Bøgelund et al. 2018) and G+0.693-0.027 systems (Zeng et al. 2023; methanol from Rodríguez-Almeida et al. 2021). Moreover, the upper limit ratios of z-cyanomethanimine and glyceraldehyde to methanol toward G+0.693-0.027 (Jiménez-Serra et al. 2020) are consistent with our upper limit ratios. However, the ratio of ethanolamine/methanol toward this source (Rivilla et al. 2021) was found to be around one order of magnitude higher than the Band 3 upper limit measurement of IRAS 16293



B. The discussed ratios in this section may be generally higher in G+0.693-0.027 than IRAS 16293 B. Given the small sample size and the upper limit nature of our results, it is not possible to draw further conclusions on the significance of these differences and similarities. This is particularly the case, because of the upper limits reported here tend to depend on the assumed excitation temperature and more importantly the lines covered in our data.

## 5. Conclusions

We analyzed the deep ALMA Band 3 (~100 GHz) data of IRAS16293 B in this work. We searched for large organic species in this dataset and derived the corresponding column densities and excitation temperatures of various oxygen-, nitrogen-, and sulfur-bearing molecules. Below are the main conclusions of this work.

- The line density for lines detected at a  $\geq 6\sigma$  level in Band 3 observations is one per ~8.5 MHz, which is only ~2.5 times lower than that of PILS: the spectrum is relatively rich and crowded even at ~3 mm observations.
- We detected around 31 molecules (including minor isotopologues), thereof ~15 tentatively, in the Band 3 dataset. These include O-bearing COMs such as CH<sub>3</sub>OH, CH<sub>2</sub>OHCHO, CH<sub>3</sub>OCH<sub>3</sub>, CH<sub>3</sub>OCHO, gGg-(CH<sub>2</sub>OH)<sub>2</sub>, CH<sub>3</sub>COCH<sub>3</sub>, and c-C<sub>2</sub>H<sub>4</sub>O. We also tentatively detected a few N- and S-bearing species such as HOCH<sub>2</sub>CN and CH<sub>3</sub>SH.
- We searched for many large COMs among which are glycerol and isopropanol, but we did not detect them. The upper limits on the 41 non-detected species are also provided, which generally agree with the previous laboratory experiments and observations.
- In the Band 3 spectrum, ~25 – 30% of all lines at the  $\geq 6\sigma$  level were not identified. This points to the need for additional spectroscopic information.
- We find good agreement between the column densities of Band 3 and Band 7 observations with a scatter of less than a factor of two. Moreover, the Band 3 ratios with respect to methanol agree within a factor of about two with those from the Band 7 observations.
- We conclude that around IRAS16293 B, the dust optical depth does not affect the column densities and the ratios of various molecules, especially for the spectrum extracted from a position off-source (where the dust column density is lower than on-source).

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Table A.1: Spectroscopic information

| Name                 | Species                                 | Catalog    | References   |
|----------------------|---|------------|--|
| Methanol             | $^{13}\text{CH}_3\text{OH}$             | CDMS       | Xu & Lovas (1997)  |
| Methanol             | $\text{CH}_2\text{DOH}$                 | JPL        | Pearson et al. (2012)  |
| Methanol             | $\text{CHD}_2\text{OH}$                 | CDMS       | Drozdzovskaya et al. (2022)  |
| Methanol             | $\text{CD}_3\text{OH}$                  | CDMS       | Ilyushin et al. (2022)   |
| Acetaldehyde         | $\text{CH}_3\text{CHO}$                 | JPL        | Kleiner et al. (1996)  |
| Acetaldehyde         | $^{13}\text{CH}_3\text{CHO}$            | CDMS       | Margulès et al. (2015)   |
| Acetaldehyde         | $\text{CH}_2\text{DCHO}$                | CDMS       | Coudert et al. (2019)  |
| Acetaldehyde         | $\text{CH}_3\text{CDO}$                 | CDMS       | Coudert et al. (2019)  |
| Acetaldehyde         | $\text{CHD}_2\text{CHO}$                | JPL format | Ferrer Asensio et al. (2023)   |
| Acetic acid          | $\text{CH}_3\text{COOH}$                | CDMS       | Ilyushin et al. (2013)   |
| Glycolaldehyde       | $\text{CH}_2\text{OHCHO}$               | CDMS       | Müller 2021, unpublished   |
| Glycolaldehyde       | $^{13}\text{CH}_2\text{OHCHO}$          | CDMS       | Haykal et al. (2013)   |
| Glycolaldehyde       | $\text{CHDOHCHO}$                       | CDMS       | Bouchez et al. (2012)  |
| Ethanol              | $\text{CH}_3\text{CH}_2\text{OH}$       | CDMS       | Pearson et al. (2008); Müller et al. (2016)  |
| Ethanol              | a-a- $\text{CH}_2\text{DCH}_2\text{OH}$ | CDMS       | Walters et al. (2015)  |
| Ethanol              | a- $\text{CH}_3\text{CHDOH}$            | CDMS       | Walters et al. (2015)  |
| Dimethyl ether       | $\text{CH}_3\text{OCH}_3$               | CDMS       | Endres et al. (2009)   |
| Methyl formate       | $\text{CH}_3\text{OCHO}$                | JPL        | Ilyushin et al. (2009)   |
| aGg'-ethylene glycol | aGg'-( $\text{CH}_2\text{OH}$ ) $_2$    | CDMS       | Christen et al. (1995); Christen & Müller (2003)                                       |
| gGg'-ethylene glycol | gGg'-( $\text{CH}_2\text{OH}$ ) $_2$    | CDMS       | Christen et al. (2001); Müller & Christen (2004)                                       |
| Formaldehyde         | $\text{D}_2\text{CO}$                   | CDMS       | Dangoisse et al. (1978); Bocquet et al. (1999)   |
| Cyanoacetylene       | HCCCN                                   | CDMS       | de Zafra (1971); Creswell et al. (1977); Yamada et al. (1995); Thorwirth et al. (2000) |
| Ethyl cyanide        | $\text{CH}_3\text{CH}_2\text{CN}$       | CDMS       | Pearson et al. 1994; Fukuyama et al. 1996; Brauer et al. 2009                          |
| Formamide            | $\text{NH}_2\text{CHO}$                 | CDMS       | Kukulich & Nelson 1971; Hirota et al. 1974; Kryvda et al. 2009; Motiyenko et al. 2012  |
| Acetone              | $\text{CH}_3\text{COCH}_3$              | JPL        | Groner et al. (2002); Ordu et al. (2019)   |
| Formic acid          | t-HCOOH                                 | CDMS       | Winnewisser et al. (2002)  |
| Ethylene oxide       | c- $\text{C}_2\text{H}_4\text{O}$       | CDMS       | Creswell & Schwendeman (1974); Hirose (1974); Medcraft et al. (2012)                   |
| Ethylene oxide       | c- $\text{C}_2\text{H}_3\text{DO}$      | CDMS       | Müller et al. (2023a)  |
| Methanethiol         | $\text{CH}_3\text{SH}$                  | CDMS       | Zakharenko et al. (2019)   |
| Glycolonitrile       | $\text{HOCH}_2\text{CN}$                | CDMS       | Margulès et al. (2017)   |

**Notes.** For acetone, we use a corrected entry (Ordu et al. 2019) for the apparent issues seen in Lykke et al. (2017).

## Appendix B: Additional plots and tables

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Figure B.1 presents the fitted models of each molecule to the Band 3 data, highlighting a number of lines that are yet to be determined. Figures B.2 and B.3 present the transitions of G<sub>n</sub>-propanol and G'Gg'gg'-Glycerol with the models determining their upper limits in orange. The total fit to the detected and tentative molecules is also shown in cyan. Figure B.4 presents the excitation temperatures when a measurement was possible for Band 3 results (PILS temperatures are shown for comparison). Figure B.5 shows the comparison of Band 3 and Band 7 beams on top of a two-dimensional Gaussian distribution, representing the spatial extents of COMs (e.g., see Jørgensen et al. 2016). This was done to examine the difference between the mean flux in the two beams, which is around 10%. Table B.1 shows the upper limits found for the molecules searched for but not detected. Table B.2 presents the covered transitions of the (tentatively) detected molecules in the data.

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## Appendix A: Spectroscopic data

The spectroscopic information are summarized in Table A.1. The vibrational correction factor is assumed as one for all molecules except for the following species. The vibrational correction factor of 1.457 was used for  $\text{CH}_2\text{DOH}$  at a temperature of 300 K (Lauvergnat et al. 2009; Jørgensen et al. 2018). For  $\text{CH}_2\text{OHCHO}$ , a factor of 2.86 was adopted at 300K to take the higher (than ground state) vibrational states into account, which were calculated in the harmonic approximation. For  $^{13}\text{CH}_2\text{OHCHO}$  and  $\text{CHDOHCHO}$ , a vibrational factor of 2.8 was used at a temperature of 300 K (Jørgensen et al. 2016). An upper limit vibrational factor of 2.824 at 300 K (Durig et al. 1975; Jørgensen et al. 2018) was assumed for a-a- $\text{CH}_2\text{DCH}_2\text{OH}$  and a- $\text{CH}_3\text{CHDOH}$ . Moreover, following Jørgensen et al. (2018), we multiplied the column densities of these two species by an additional factor of  $\sim 2.69$  to account for the presence of the gauche conformer. We assumed a vibration correction factor of 4.02 for aGg-( $\text{CH}_2\text{OH}$ ) $_2$  and gGg-( $\text{CH}_2\text{OH}$ ) $_2$  and added an additional factor of  $\sim 1.38$  to include the contribution from the higher gGg conformer at 300 K (Müller & Christen 2004; Jørgensen et al. 2016). A vibrational correction factor of 1.09 at 100 K was used for HCCCN (Mallinson & Fayt 1976; Calcutt et al. 2018b). For  $\text{CH}_3\text{CH}_2\text{CN}$ , a vibrational correction factor of 1.113 was assumed at 100 K. A vibrational correction factor of 1.5 was assumed for  $\text{NH}_2\text{CHO}$  at 300 K. For t-HCOOH, a vibrational correction factor of 1.103 at 300 K was assumed (Perrin et al. 2002; Baskakov et al. 2006; Jørgensen et al. 2018).

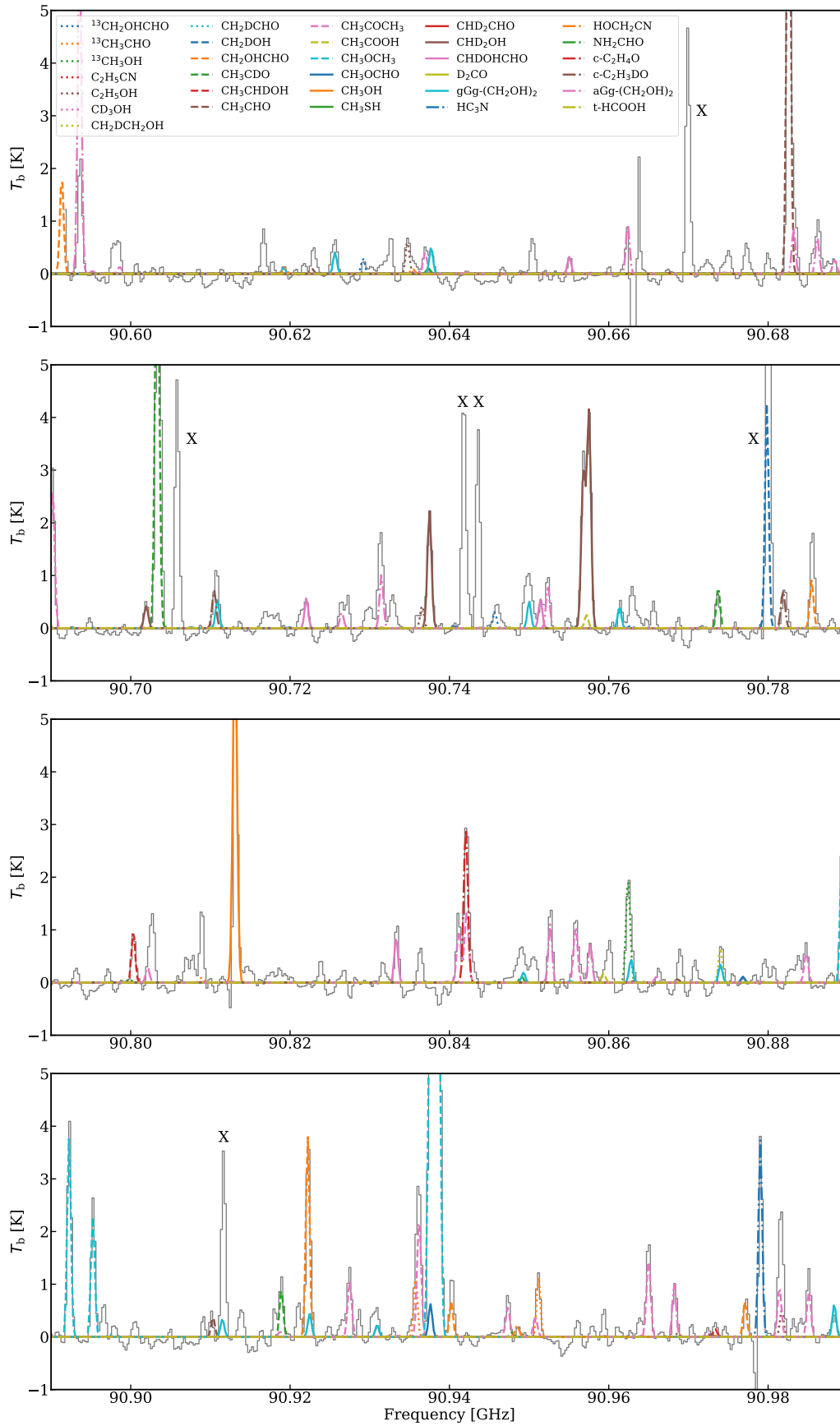


Fig. B.1: Fitted model for each molecule on top of the Band 3 data in gray. For readability, the y-axis limit was set to 5 K; however, no line was overestimated except those of methanol and one line of  $\text{aGg}'-(\text{CH}_2\text{OH})_2$ , which are potentially optically thick. The lines that have an intensity higher than 2 K (i.e., detected at a  $\geq 7 - 10\sigma$  level) but that were not identified are indicated by an "X".

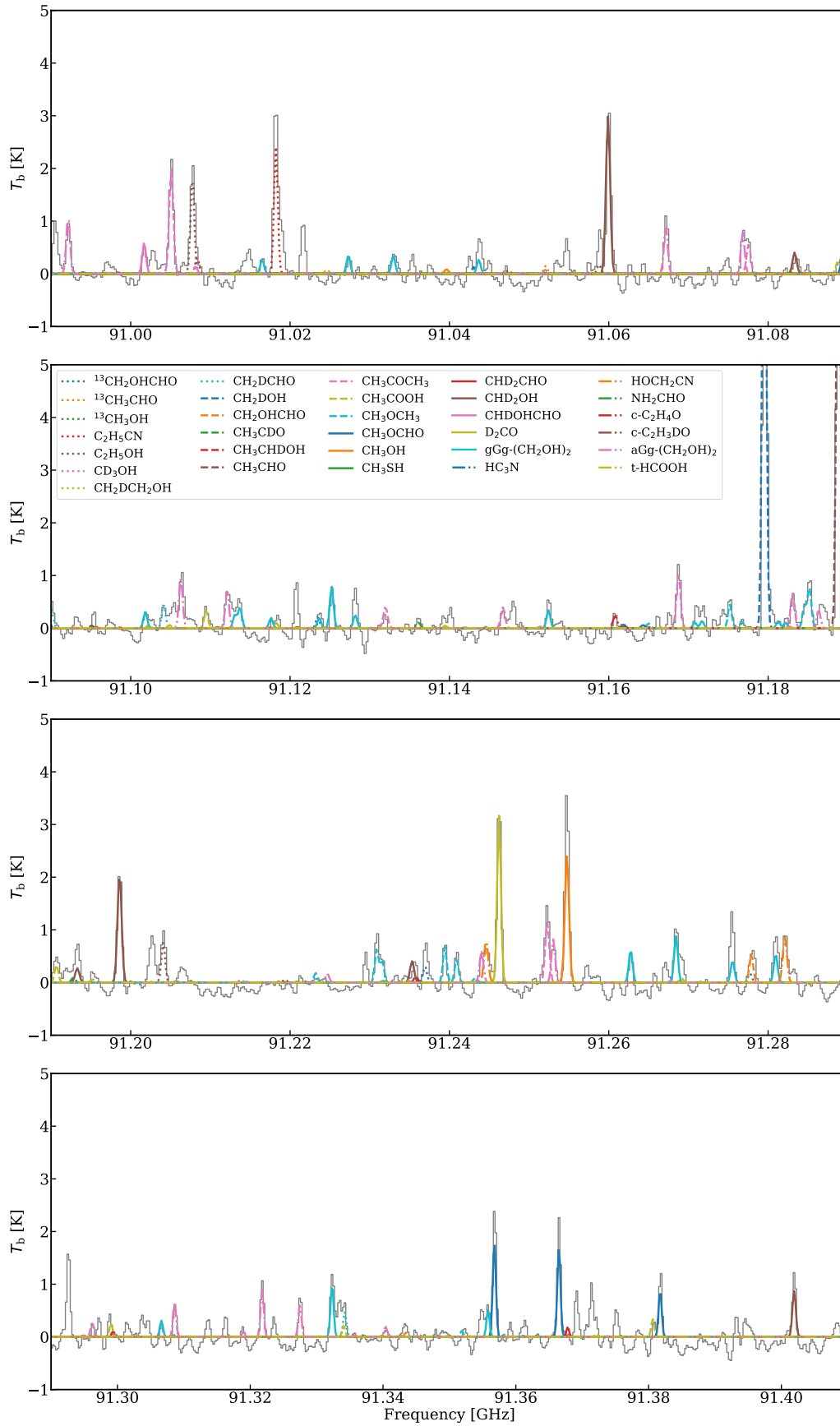


Fig. B.1: Continued



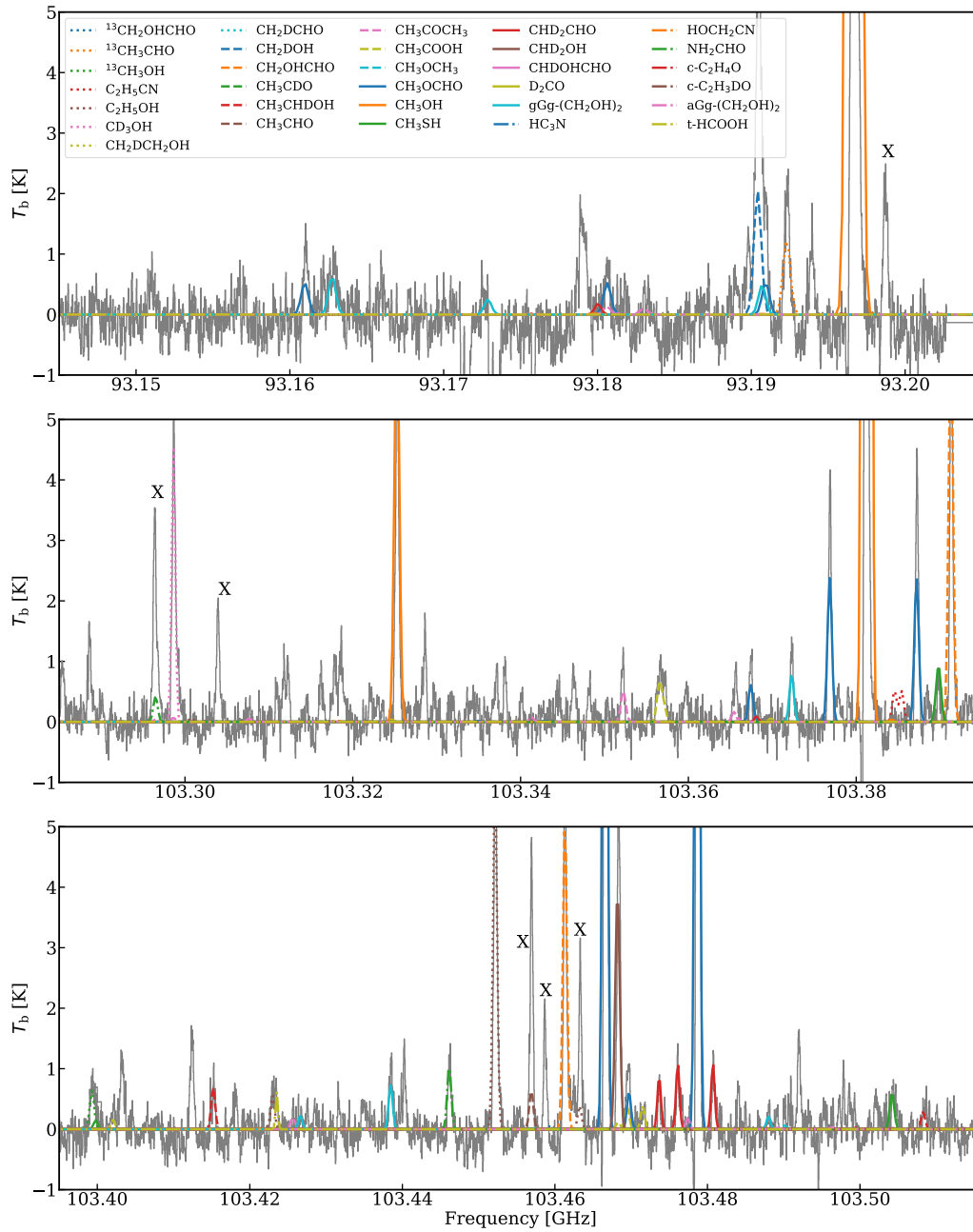


Fig. B.1: Continued

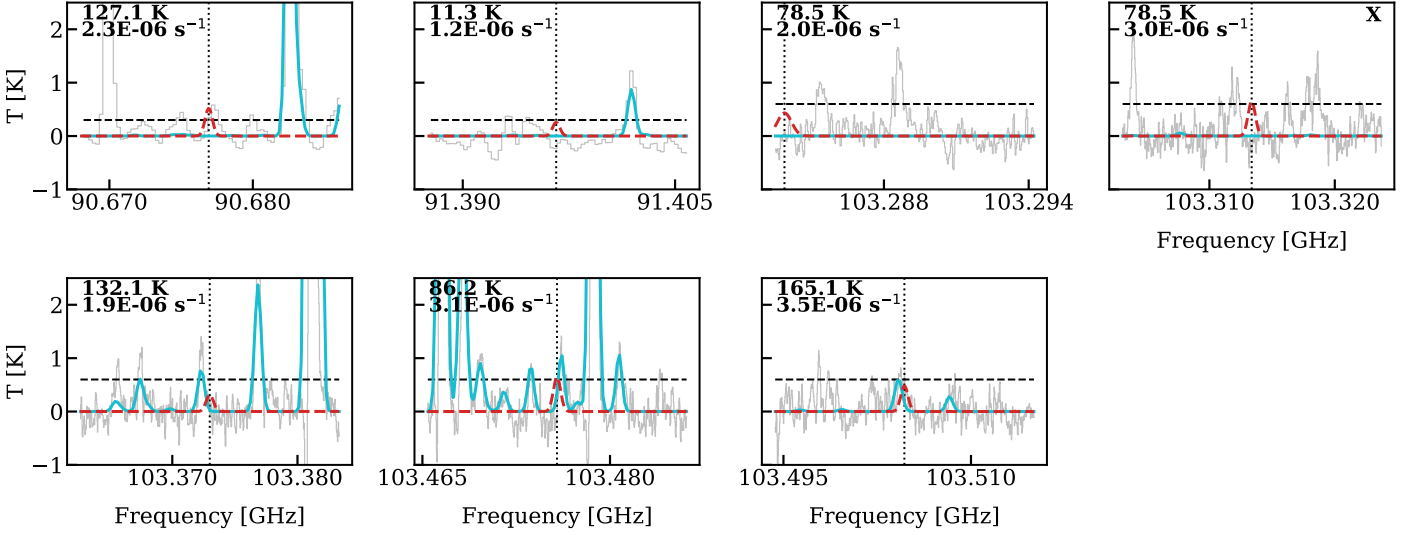


Fig. B.2: Lines of Ga-n-propanol and the model for its upper limit ( $6 \times 10^{15} \text{ cm}^{-2}$ ) in red. The symbols are the same as in Fig. 3.

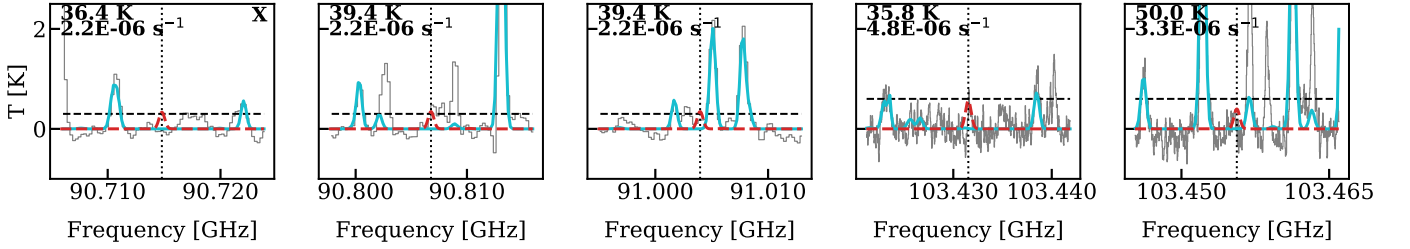


Fig. B.3: Lines of G'Gg'gg'-Glycerol and the model for its upper limit ( $7 \times 10^{15} \text{ cm}^{-2}$ ) in red. The symbols are the same as in Fig. 3.

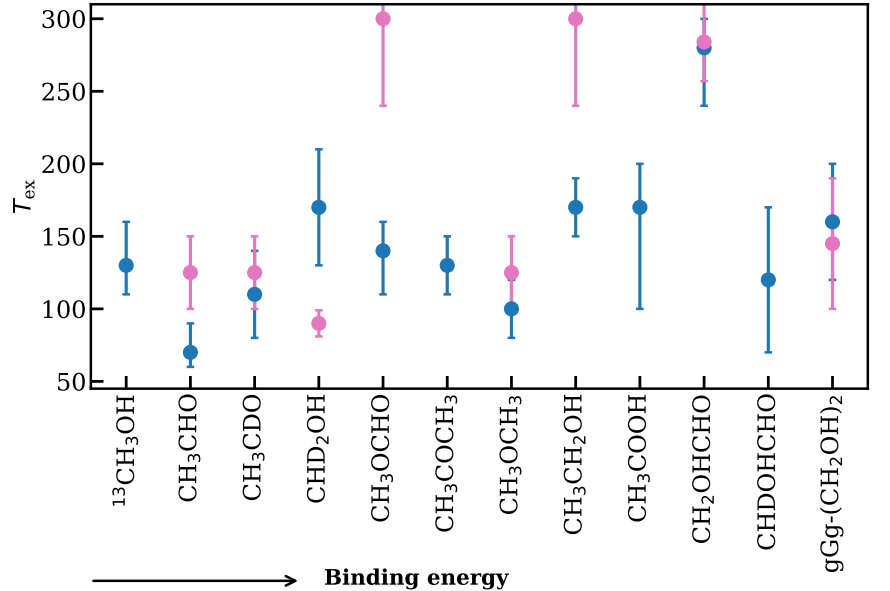


Fig. B.4: Excitation temperatures for molecules where a determination was possible. The species are ordered by their binding energies taken from Minissale et al. (2022) and Ligterink & Minissale (2023). The binding energy of the isotopologues was assumed to be the same as the major isotopologue. Band 3 results are shown in blue and Band 7 (PILS) in pink. PILS results with a fixed temperature are not shown. The temperatures for molecules from Jørgensen et al. (2018) are shown with either  $300 \pm 60 \text{ K}$  or  $125 \pm 25 \text{ K}$  depending on the group with which they were associated.

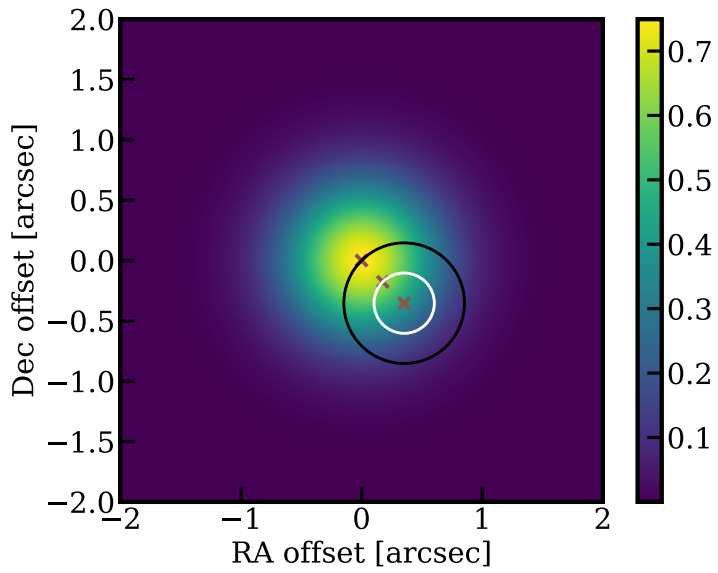


Fig. B.5: Two-dimensional Gaussian function with a total integration of one and a FWHM of  $0.5''$  (color scale). This was assumed as a typical emission distribution for COMs based on the results of PILS (e.g., [Jørgensen et al. 2016](#)). Two circular regions with radii of  $0.25''$  and  $0.5''$  are overplotted, representing beams of PILS (white) and Band 3 (black), respectively. The crosses show the peak position,  $0.25''$ , and  $0.5''$  offset positions.



Table B.1: Upper limits of non-detections.

| Name                        | Molecular formula   | Upper limit ( $\text{cm}^{-2}$ ) |
|-----------------------------|---|----------------------------------|
| Methanol                    | $\text{CH}_3^{18}\text{OH}$                                       | $<5.0 \times 10^{17}$            |
| Formamide                   | $\text{NH}_2\text{CDO}$   | $<2.0 \times 10^{15}$            |
| Formamide                   | $\text{NH}_2^{13}\text{CHO}$                                      | $<1.2 \times 10^{16}$            |
| Formamide                   | cis-NHDCHO  | $<2.5 \times 10^{15}$            |
| Formamide                   | trans-NHDCHO  | $<5.0 \times 10^{15}$            |
| Formamide                   | $\text{NH}_2\text{CHO}(v_{12} = 1)$                               | $<5.0 \times 10^{17}$            |
| Z-cyanomethanimine          | Z-HNCHCN  | $<5.5 \times 10^{15}$            |
| Methanethiol                | $^{13}\text{CH}_3\text{SH}$                                       | $<7.0 \times 10^{15}$            |
| Cyanodiacetylene            | $\text{HC}_5\text{N}$   | $<2.0 \times 10^{13}$            |
| Ethylene oxide              | c- $\text{CD}_2\text{CH}_2\text{O}$                               | $<6.0 \times 10^{14}$            |
| Acetaldehyde                | $\text{CH}_3^{13}\text{CHO}$                                      | $<6.0 \times 10^{15}$            |
| Vinyl cyanide               | $\text{C}_2\text{H}_3\text{CN}$                                   | $<4.0 \times 10^{15}$            |
| Glycolaldehyde              | $\text{CH}_2\text{OHCDO}$   | $<1.0 \times 10^{15}$            |
| Glycolaldehyde              | $\text{CH}_2\text{ODCHO}$   | $<5.0 \times 10^{14}$            |
| Glycolaldehyde              | $\text{CH}_2\text{OH}^{13}\text{CHO}$                             | $<1.5 \times 10^{15}$            |
| Methyl formate              | $\text{CH}_3\text{O}^{13}\text{CHO}$                              | $<7.0 \times 10^{15}$            |
| Propargyl cyanide           | $\text{HCCCH}_2\text{CN}$   | $<7.0 \times 10^{14}$            |
| Propenal                    | $\text{C}_2\text{H}_3\text{CHO}$                                  | $<1.5 \times 10^{14}$            |
| Protonated cyanodiacetylene | $\text{HC}_5\text{NH}^+$  | $<1.5 \times 10^{13}$            |
| Urea                        | $\text{H}_2\text{NCONH}_2$  | $<1.5 \times 10^{14}$            |
| Ethanol                     | a- $^{13}\text{CH}_3\text{CH}_2\text{OH}$                         | $<8.0 \times 10^{14}$            |
| Ethanol                     | a- $\text{CH}_3^{13}\text{CH}_2\text{OH}$                         | $<1.5 \times 10^{18}$            |
| Ethanol                     | a- $\text{CH}_3\text{CH}_2\text{OD}$                              | $<1.0 \times 10^{15}$            |
| Ethanol                     | a-s- $\text{CH}_2\text{DCH}_2\text{OH}$                           | $<3.0 \times 10^{15}$            |
| Gauche-ethyl mercaptan      | g- $\text{C}_2\text{H}_5\text{SH}$                                | $<1.0 \times 10^{15}$            |
| Methoxymethanol             | $\text{CH}_3\text{OCH}_2\text{OH}$                                | $<4.0 \times 10^{17}$            |
| s-propanal                  | s- $\text{C}_2\text{H}_5\text{CHO}$                               | $<1.5 \times 10^{15}$            |
| g-propanal                  | g- $\text{C}_2\text{H}_5\text{CHO}$                               | $<3.5 \times 10^{17}$            |
| Cyclopentadiene             | c- $\text{C}_5\text{H}_6$   | $<5.0 \times 10^{16}$            |
| Ethanolamine                | $\text{NH}_2\text{CH}_2\text{CH}_2\text{OH}$                      | $<6.0 \times 10^{14}$            |
| Ga-n-propanol               | Ga-n- $\text{C}_3\text{H}_7\text{OH}$                             | $<6.0 \times 10^{15}$            |
| Glyceraldehyde              | $\text{HCOCHOHCH}_2\text{OH}$                                     | $<8.0 \times 10^{15}$            |
| g-Isopropanol               | g-i- $\text{C}_3\text{H}_7\text{OH}$                              | $<1.5 \times 10^{16}$            |
| a-Isopropanol               | a-i- $\text{C}_3\text{H}_7\text{OH}$                              | $<2.0 \times 10^{16}$            |
| Benzonitrile                | c- $\text{C}_6\text{H}_5\text{CN}$                                | $<1.0 \times 10^{14}$            |
| Benzaldehyde                | c- $\text{C}_6\text{H}_5\text{CHO}$                               | $<7.0 \times 10^{14}$            |
| GGag'g'-Glycerol            | GGag'g'- $\text{HOCH}_2\text{CH}(\text{OH})\text{CH}_2\text{OH}$  | $<8.0 \times 10^{14}$            |
| G'Gg'gg'-Glycerol           | G'Gg'gg'- $\text{HOCH}_2\text{CH}(\text{OH})\text{CH}_2\text{OH}$ | $<7.0 \times 10^{15}$            |
| Indene                      | c- $\text{C}_9\text{H}_8$   | $<1.0 \times 10^{16}$            |
| 1-cyanonaphthalene          | 1- $\text{C}_{10}\text{H}_7\text{CN}$                             | $<1.0 \times 10^{14}$            |
| 2-cyanonaphthalene          | 2- $\text{C}_{10}\text{H}_7\text{CN}$                             | $<2.0 \times 10^{14}$            |

**Notes.** Upper limits on column densities toward the  $0.5''$  offset position from source B in a  $\sim 1''$  beam. If a source size of  $0.5''$  was assumed, these values would increase by a factor of  $\sim 5$ . The upper limits are measured by fixing  $T_{\text{ex}}$  to 100 K and FWHM to  $2 \text{ km s}^{-1}$ . Vibrational correction factors are not included in these values.

Table B.2: Transitions of the species studied here in the data that have  $E_{\text{up}} < 1000$  K and  $A_{ij} > 10^{-9} \text{ s}^{-1}$  (not all were detected).

| Species                          | Transition<br>J K L M   | Frequency<br>(MHz)    | $A_{ij}$<br>( $\text{s}^{-1}$ ) | $E_{\text{up}}$<br>(K) |
|----------------------------------|-------------------------|-----------------------|---------------------------------|------------------------|
| CH <sub>3</sub> OH               | 20 3 18 5 - 19 2 18 5   | 90 813.078            | $2.80 \times 10^{-6}$           | 808.3                  |
|                                  | 20 2 18 2 - 20 2 19 1   | 91 254.751            | $5.29 \times 10^{-8}$           | 514.3                  |
|                                  | 1 0 1 4 - 2 1 2 4       | 93 196.672            | $4.19 \times 10^{-6}$           | 302.9                  |
|                                  | 12 3 10 1 - 13 0 13 1   | 103 325.252           | $1.81 \times 10^{-8}$           | 228.8                  |
|                                  | 12 2 10 2 - 12 1 11 1   | 103 381.258           | $3.98 \times 10^{-7}$           | 207.1                  |
| <sup>13</sup> CH <sub>3</sub> OH | 18 -4 15 0 - 17 -5 12 0 | 90 862.42             | $1.17 \times 10^{-6}$           | 475.4                  |
|                                  | 8 -2 7 0 - 8 1 7 0      | 103 399.296           | $6.15 \times 10^{-8}$           | 107.6                  |
| CH <sub>2</sub> DOH              | 22 3 19 0 - 21 4 17 2   | 90 762.771            | $5.43 \times 10^{-8}$           | 580.9                  |
|                                  | 2 1 1 0 - 1 1 0 0       | 90 779.841            | $1.57 \times 10^{-6}$           | 10.6                   |
|                                  | 25 0 25 1 - 24 3 21 2   | 91 043.068            | $2.77 \times 10^{-7}$           | 702.0                  |
|                                  | 9 1 8 1 - 9 0 9 1       | 91 179.518            | $2.06 \times 10^{-6}$           | 113.9                  |
|                                  | 29 2 28 1 - 28 4 24 2   | 91 392.257            | $1.91 \times 10^{-8}$           | 955.2                  |
|                                  | 28 3 25 0 - 28 3 26 0   | 91 395.302            | $9.47 \times 10^{-8}$           | 911.8                  |
|                                  | 18 4 14 0 - 17 5 13 0   | 93 190.407            | $1.27 \times 10^{-6}$           | 430.1                  |
|                                  | 26 1 25 1 - 25 4 22 1   | 93 193.888            | $2.35 \times 10^{-9}$           | 772.1                  |
|                                  | 18 6 12 2 - 18 6 12 1   | 103 347.889           | $1.51 \times 10^{-9}$           | 522.9                  |
|                                  | 18 6 13 2 - 18 6 13 1   | 103 347.925           | $1.51 \times 10^{-9}$           | 522.9                  |
| CHD <sub>2</sub> OH              | 10 3 2 1 - 11 0 2 1     | 90 701.939            | $5.61 \times 10^{-8}$           | 144.1                  |
|                                  | 20 4 1 1 - 20 4 2 0     | 90 717.394            | $1.02 \times 10^{-9}$           | 474.9                  |
|                                  | 18 4 2 0 - 18 3 1 2     | 90 737.495            | $7.34 \times 10^{-7}$           | 392.4                  |
|                                  | 10 4 2 1 - 11 3 2 0     | 90 756.808            | $4.52 \times 10^{-7}$           | 165.0                  |
|                                  | 10 2 1 2 - 9 3 1 2      | 90 757.511            | $5.45 \times 10^{-7}$           | 141.1                  |
|                                  | 2 1 1 2 - 3 1 1 1       | 90 767.952            | $1.35 \times 10^{-9}$           | 27.7                   |
|                                  | 8 2 1 0 - 8 0 2 1       | 90 863.187            | $3.73 \times 10^{-9}$           | 84.9                   |
|                                  | 6 2 1 2 - 7 2 1 0       | 90 945.187            | $1.94 \times 10^{-9}$           | 73.2                   |
|                                  | 12 0 1 2 - 12 2 2 0     | 90 972.887            | $6.69 \times 10^{-9}$           | 173.9                  |
|                                  | 10 4 1 1 - 11 3 1 0     | 91 059.907            | $4.61 \times 10^{-7}$           | 165.0                  |
|                                  | 22 5 1 0 - 21 6 1 1     | 91 083.326            | $3.39 \times 10^{-7}$           | 583.4                  |
|                                  | 24 0 1 0 - 23 3 1 1     | 91 110.901            | $1.39 \times 10^{-8}$           | 590.9                  |
|                                  | 18 10 1 0 - 19 9 1 2    | 91 193.289            | $2.03 \times 10^{-7}$           | 647.5                  |
|                                  | 18 10 2 0 - 19 9 2 2    | 91 193.289            | $2.03 \times 10^{-7}$           | 647.5                  |
|                                  | 18 4 1 0 - 18 3 2 2     | 91 198.598            | $6.93 \times 10^{-7}$           | 392.4                  |
|                                  | 22 5 2 0 - 21 6 2 1     | 91 235.311            | $3.40 \times 10^{-7}$           | 583.5                  |
|                                  | 12 2 2 0 - 12 1 1 1     | 91 401.917            | $1.16 \times 10^{-7}$           | 169.5                  |
|                                  | 10 3 1 2 - 11 2 1 1     | 103 468.208           | $7.46 \times 10^{-7}$           | 156.7                  |
| 6 1 2 2 - 7 1 2 0                | 103 504.343             | $3.22 \times 10^{-9}$ | 63.3                            |                        |
| CD <sub>3</sub> OH               | 10 4 6 1 - 11 3 8 1     | 103 298.627           | $1.47 \times 10^{-6}$           | 156.5                  |
| CH <sub>3</sub> CHO              | 25 3 23 3 - 26 0 26 3   | 90 618.941            | $2.12 \times 10^{-8}$           | 526.0                  |
|                                  | 7 3 5 4 - 8 2 7 4       | 90 622.765            | $5.86 \times 10^{-7}$           | 250.3                  |
|                                  | 4 2 3 1 - 5 0 5 2       | 90 636.495            | $3.21 \times 10^{-9}$           | 18.3                   |
|                                  | 34 4 30 8 - 35 2 34 7   | 90 670.793            | $8.13 \times 10^{-9}$           | 970.9                  |
|                                  | 11 1 10 2 - 11 0 11 2   | 90 682.574            | $3.14 \times 10^{-6}$           | 64.9                   |
|                                  | 28 5 23 3 - 29 3 26 3   | 90 723.537            | $1.86 \times 10^{-8}$           | 636.9                  |
|                                  | 31 2 29 0 - 32 0 32 0   | 90 730.219            | $2.82 \times 10^{-9}$           | 475.7                  |
|                                  | 13 2 11 6 - 14 1 14 6   | 90 731.485            | $6.83 \times 10^{-7}$           | 471.1                  |
|                                  | 37 4 33 5 - 37 4 34 4   | 90 737.826            | $3.52 \times 10^{-7}$           | 897.9                  |
|                                  | 21 6 15 5 - 22 5 17 5   | 90 743.918            | $6.78 \times 10^{-7}$           | 500.7                  |
|                                  | 35 4 32 4 - 36 2 35 4   | 90 746.919            | $3.37 \times 10^{-9}$           | 825.9                  |
|                                  | 29 3 27 4 - 29 2 27 5   | 90 791.888            | $1.23 \times 10^{-9}$           | 628.4                  |
|                                  | 21 2 19 6 - 22 1 22 6   | 90 856.686            | $3.05 \times 10^{-7}$           | 604.1                  |
|                                  | 9 0 9 5 - 8 1 7 5       | 90 868.634            | $2.84 \times 10^{-7}$           | 245.7                  |
|                                  | 28 2 26 2 - 27 4 23 2   | 90 905.459            | $2.57 \times 10^{-8}$           | 391.5                  |
|                                  | 5 0 5 8 - 4 0 4 8       | 90 910.33             | $2.42 \times 10^{-5}$           | 391.6                  |
|                                  | 24 4 20 8 - 24 4 21 7   | 90 999.685            | $4.68 \times 10^{-8}$           | 693.0                  |
|                                  | 40 5 36 0 - 41 2 39 0   | 91 005.733            | $6.98 \times 10^{-8}$           | 817.0                  |
|                                  | 17 2 16 3 - 16 3 13 3   | 91 095.085            | $5.97 \times 10^{-7}$           | 355.3                  |

Table B.2: continued.

| Species                      | Transition<br>J K L M   | Frequency<br>(MHz) | $A_{ij}$<br>( $s^{-1}$ ) | $E_{up}$<br>(K) |
|------------------------------|-------------------------|--------------------|--------------------------|-----------------|
|                              | 30 3 28 7 - 31 0 31 8   | 91 155.32          | $5.90 \times 10^{-9}$    | 829.2           |
|                              | 11 1 10 0 - 11 0 11 0   | 91 188.823         | $3.22 \times 10^{-6}$    | 64.8            |
|                              | 36 4 33 4 - 37 2 36 4   | 91 189.824         | $3.10 \times 10^{-9}$    | 859.3           |
|                              | 34 4 31 4 - 35 2 34 4   | 91 213.789         | $3.73 \times 10^{-9}$    | 793.4           |
|                              | 31 5 27 0 - 30 6 24 0   | 91 296.802         | $7.77 \times 10^{-7}$    | 516.1           |
|                              | 20 1 19 8 - 19 3 17 7   | 93 202.965         | $6.38 \times 10^{-9}$    | 581.1           |
|                              | 33 4 30 1 - 34 2 33 1   | 103 321.687        | $1.06 \times 10^{-8}$    | 556.4           |
|                              | 5 2 4 7 - 4 1 3 8       | 103 326.134        | $2.76 \times 10^{-9}$    | 401.5           |
|                              | 33 2 32 0 - 32 3 29 0   | 103 354.087        | $1.84 \times 10^{-7}$    | 520.8           |
|                              | 34 4 31 1 - 35 2 34 1   | 103 378.41         | $1.03 \times 10^{-8}$    | 587.9           |
|                              | 32 2 30 5 - 33 0 33 5   | 103 395.991        | $3.64 \times 10^{-9}$    | 711.1           |
|                              | 36 5 32 1 - 37 3 35 1   | 103 429.039        | $1.42 \times 10^{-8}$    | 674.0           |
|                              | 11 2 9 3 - 11 1 10 3    | 103 456.903        | $4.86 \times 10^{-6}$    | 275.9           |
|                              | 30 8 23 3 - 31 7 24 3   | 103 489.605        | $9.90 \times 10^{-7}$    | 779.4           |
|                              | 30 8 22 3 - 31 7 25 3   | 103 496.344        | $9.90 \times 10^{-7}$    | 779.4           |
| $^{13}\text{CH}_3\text{CHO}$ | 37 6 32 -3 - 36 7 29 -3 | 90 765.097         | $7.94 \times 10^{-7}$    | 918.8           |
|                              | 27 7 21 -3 - 28 6 22 -3 | 90 791.095         | $7.33 \times 10^{-7}$    | 655.2           |
|                              | 16 2 14 1 - 15 3 12 1   | 90 802.2           | $6.92 \times 10^{-8}$    | 132.8           |
|                              | 27 7 20 -3 - 28 6 23 -3 | 90 830.059         | $7.34 \times 10^{-7}$    | 655.2           |
|                              | 22 3 20 -3 - 23 0 23 -3 | 90 904.355         | $2.60 \times 10^{-8}$    | 452.6           |
|                              | 5 1 5 0 - 4 1 4 0       | 90 935.753         | $2.41 \times 10^{-5}$    | 15.4            |
|                              | 5 1 5 1 - 4 1 4 1       | 90 951.18          | $2.41 \times 10^{-5}$    | 15.4            |
|                              | 33 4 30 -3 - 34 2 33 -3 | 90 961.839         | $1.73 \times 10^{-8}$    | 746.1           |
|                              | 5 1 5 -3 - 4 1 4 -3     | 91 052.078         | $2.44 \times 10^{-5}$    | 221.8           |
|                              | 34 4 31 -3 - 35 2 34 -3 | 91 058.163         | $1.68 \times 10^{-8}$    | 776.8           |
|                              | 29 2 27 -2 - 28 4 24 -2 | 91 172.915         | $1.78 \times 10^{-8}$    | 612.2           |
|                              | 25 3 23 -3 - 26 0 26 -3 | 91 232.409         | $2.32 \times 10^{-8}$    | 517.4           |
|                              | 29 3 26 -3 - 29 3 27 -3 | 91 304.282         | $6.05 \times 10^{-7}$    | 620.5           |
|                              | 5 2 4 1 - 4 2 2 1       | 91 305.92          | $1.01 \times 10^{-7}$    | 22.5            |
|                              | 23 1 22 1 - 22 3 19 1   | 91 313.98          | $3.30 \times 10^{-8}$    | 253.5           |
|                              | 32 5 28 0 - 31 6 25 0   | 91 370.438         | $8.31 \times 10^{-7}$    | 531.6           |
|                              | 11 2 10 -2 - 11 1 10 -2 | 91 386.732         | $7.84 \times 10^{-7}$    | 272.2           |
|                              | 39 5 35 0 - 40 3 38 0   | 91 395.629         | $8.97 \times 10^{-9}$    | 758.9           |
|                              | 36 9 27 -3 - 37 8 29 -3 | 93 187.027         | $8.16 \times 10^{-7}$    | 985.7           |
|                              | 5 0 5 1 - 4 0 4 1       | 93 192.298         | $2.70 \times 10^{-5}$    | 13.5            |
|                              | 36 9 28 -3 - 37 8 30 -3 | 93 194.864         | $8.16 \times 10^{-7}$    | 985.7           |
|                              | 39 4 36 -3 - 40 2 39 -3 | 103 353.904        | $2.05 \times 10^{-8}$    | 943.5           |
|                              | 18 3 16 -3 - 19 0 19 -3 | 103 463.152        | $4.01 \times 10^{-8}$    | 378.7           |
|                              | 38 5 34 -2 - 39 2 37 -2 | 103 484.196        | $7.87 \times 10^{-8}$    | 928.7           |
|                              | 12 2 10 -3 - 12 1 11 -3 | 103 487.851        | $5.26 \times 10^{-6}$    | 285.2           |
| $\text{CH}_3\text{CDO}$      | 5 1 5 0 - 4 1 4 0       | 90 703.205         | $2.39 \times 10^{-5}$    | 14.8            |
|                              | 5 1 5 1 - 4 1 4 1       | 90 703.424         | $2.39 \times 10^{-5}$    | 14.8            |
|                              | 16 3 13 5 - 15 4 12 4   | 90 707.948         | $5.88 \times 10^{-8}$    | 341.0           |
|                              | 5 1 5 3 - 4 1 4 3       | 90 773.736         | $2.41 \times 10^{-5}$    | 216.4           |
|                              | 4 2 2 3 - 4 1 3 3       | 90 799.825         | $2.55 \times 10^{-6}$    | 217.0           |
|                              | 22 2 21 1 - 21 3 18 2   | 90 823.11          | $2.02 \times 10^{-7}$    | 232.9           |
|                              | 10 1 9 5 - 10 0 10 5    | 90 849.045         | $2.77 \times 10^{-6}$    | 253.5           |
|                              | 8 2 6 0 - 8 1 7 0       | 90 918.912         | $3.66 \times 10^{-6}$    | 39.8            |
|                              | 14 3 12 3 - 15 0 15 3   | 90 926.592         | $2.93 \times 10^{-8}$    | 311.4           |
|                              | 17 2 16 1 - 16 3 13 2   | 90 947.817         | $4.54 \times 10^{-7}$    | 144.3           |
|                              | 11 5 6 2 - 12 4 8 2     | 91 192.805         | $5.21 \times 10^{-7}$    | 102.6           |
|                              | 15 2 14 4 - 14 3 12 4   | 91 214.539         | $3.12 \times 10^{-7}$    | 315.3           |
|                              | 22 8 14 5 - 23 7 16 5   | 91 278.766         | $6.04 \times 10^{-7}$    | 539.7           |
|                              | 25 12 13 2 - 24 6 19 4  | 103 300.073        | $9.11 \times 10^{-7}$    | 539.8           |
|                              | 16 11 6 1 - 15 3 13 4   | 103 316.694        | $3.40 \times 10^{-7}$    | 329.6           |
|                              | 2 2 1 4 - 2 1 2 4       | 103 470.435        | $2.49 \times 10^{-6}$    | 209.1           |

Table B.2: continued.

| Species                            | Transition<br>J K L M   | Frequency<br>(MHz)    | $A_{ij}$<br>( $s^{-1}$ ) | $E_{up}$<br>(K)       |
|------------------------------------|-------------------------|-----------------------|--------------------------|-----------------------|
| CH <sub>2</sub> DCHO               | 6 3 4 2 - 7 2 6 1       | 90 671.76             | $1.70 \times 10^{-7}$    | 59.2                  |
|                                    | 5 2 3 1 - 4 2 3 2       | 90 897.364            | $4.40 \times 10^{-7}$    | 43.7                  |
|                                    | 5 2 3 2 - 4 2 3 1       | 90 979.724            | $2.97 \times 10^{-7}$    | 43.7                  |
|                                    | 3 1 3 0 - 2 0 2 0       | 91 090.016            | $3.43 \times 10^{-6}$    | 7.0                   |
|                                    | 13 1 12 2 - 13 0 13 2   | 91 104.13             | $3.02 \times 10^{-6}$    | 104.7                 |
|                                    | 18 2 16 0 - 18 2 17 0   | 91 308.321            | $5.09 \times 10^{-7}$    | 162.7                 |
|                                    | 13 1 12 1 - 13 0 13 1   | 91 334.229            | $3.06 \times 10^{-6}$    | 104.6                 |
|                                    | 6 3 4 1 - 7 2 6 2       | 91 344.243            | $5.69 \times 10^{-8}$    | 59.3                  |
|                                    | 25 8 18 0 - 26 7 19 0   | 103 303.817           | $1.11 \times 10^{-6}$    | 409.4                 |
|                                    | 25 8 17 0 - 26 7 20 0   | 103 308.431           | $1.11 \times 10^{-6}$    | 409.4                 |
|                                    | 16 4 12 0 - 17 2 15 0   | 103 450.4             | $1.69 \times 10^{-8}$    | 151.2                 |
|                                    | 11 2 10 1 - 11 1 10 2   | 103 463.833           | $1.35 \times 10^{-8}$    | 87.7                  |
|                                    | CHD <sub>2</sub> CHO    | 6 1 5 2 - 5 1 4 2     | 103 473.67               | $3.75 \times 10^{-9}$ |
| 6 0 6 1 - 5 0 5 1                  |                         | 103 476.11            | $3.72 \times 10^{-9}$    | 17.4                  |
| 6 0 6 0 - 5 0 5 0                  |                         | 103 480.72            | $3.72 \times 10^{-9}$    | 17.4                  |
| CH <sub>3</sub> CH <sub>2</sub> OH | 39 13 27 1 - 38 14 25 0 | 90 616.41             | $4.90 \times 10^{-7}$    | 916.5                 |
|                                    | 39 13 26 1 - 38 14 24 0 | 90 616.41             | $4.90 \times 10^{-7}$    | 916.5                 |
|                                    | 39 3 36 1 - 39 4 36 0   | 90 634.74             | $5.11 \times 10^{-6}$    | 728.3                 |
|                                    | 47 1 46 2 - 46 1 46 1   | 90 673.782            | $1.70 \times 10^{-8}$    | 916.6                 |
|                                    | 47 1 46 2 - 46 0 46 1   | 90 673.816            | $3.95 \times 10^{-8}$    | 916.6                 |
|                                    | 47 2 46 2 - 46 1 46 1   | 90 674.536            | $3.95 \times 10^{-8}$    | 916.6                 |
|                                    | 47 2 46 2 - 46 0 46 1   | 90 674.571            | $1.70 \times 10^{-8}$    | 916.6                 |
|                                    | 42 5 38 1 - 43 5 38 2   | 90 701.878            | $1.88 \times 10^{-8}$    | 844.8                 |
|                                    | 31 8 24 2 - 30 6 24 1   | 90 724.54             | $2.48 \times 10^{-8}$    | 497.7                 |
|                                    | 28 12 17 2 - 29 11 18 2 | 90 736.55             | $7.33 \times 10^{-7}$    | 521.5                 |
|                                    | 28 12 16 2 - 29 11 19 2 | 90 736.571            | $7.33 \times 10^{-7}$    | 521.5                 |
|                                    | 38 6 33 1 - 39 7 33 2   | 90 809.192            | $1.68 \times 10^{-8}$    | 724.0                 |
|                                    | 19 3 16 1 - 19 2 17 1   | 90 824.709            | $5.78 \times 10^{-8}$    | 232.3                 |
|                                    | 21 20 1 2 - 21 19 2 0   | 90 947.962            | $6.04 \times 10^{-8}$    | 694.1                 |
|                                    | 21 20 2 2 - 21 19 3 0   | 90 947.962            | $6.04 \times 10^{-8}$    | 694.1                 |
|                                    | 21 2 19 1 - 21 2 19 0   | 90 968.68             | $7.21 \times 10^{-8}$    | 262.0                 |
|                                    | 7 2 6 1 - 6 3 4 0       | 90 981.716            | $5.24 \times 10^{-7}$    | 89.7                  |
|                                    | 29 2 27 1 - 29 7 23 2   | 90 992.97             | $8.40 \times 10^{-8}$    | 432.1                 |
|                                    | 14 2 13 2 - 13 3 10 2   | 91 007.739            | $9.91 \times 10^{-7}$    | 92.6                  |
|                                    | 36 10 27 1 - 35 11 24 1 | 91 030.651            | $3.31 \times 10^{-8}$    | 737.8                 |
|                                    | 36 10 26 1 - 35 11 25 1 | 91 030.969            | $3.31 \times 10^{-8}$    | 737.8                 |
|                                    | 18 3 15 1 - 18 2 16 1   | 91 047.417            | $5.85 \times 10^{-8}$    | 216.2                 |
|                                    | 25 2 24 2 - 24 3 21 2   | 91 058.798            | $1.52 \times 10^{-7}$    | 272.8                 |
|                                    | 25 11 15 2 - 26 10 16 2 | 91 204.078            | $8.20 \times 10^{-7}$    | 424.7                 |
|                                    | 25 11 14 2 - 26 10 17 2 | 91 204.079            | $8.20 \times 10^{-7}$    | 424.7                 |
|                                    | 20 3 17 1 - 20 3 17 0   | 91 219.35             | $5.52 \times 10^{-8}$    | 249.4                 |
|                                    | 7 2 6 0 - 7 1 7 0       | 91 241.609            | $7.12 \times 10^{-9}$    | 84.9                  |
|                                    | 30 3 28 2 - 31 0 31 2   | 91 250.931            | $1.83 \times 10^{-8}$    | 399.7                 |
|                                    | 38 16 22 1 - 38 16 22 0 | 91 332.886            | $8.06 \times 10^{-8}$    | 990.3                 |
|                                    | 38 16 23 1 - 38 16 23 0 | 91 332.886            | $8.06 \times 10^{-8}$    | 990.3                 |
|                                    | 31 8 23 2 - 30 6 25 1   | 93 145.898            | $3.66 \times 10^{-8}$    | 497.7                 |
|                                    | 35 10 26 2 - 34 9 25 0  | 93 180.157            | $6.27 \times 10^{-9}$    | 655.1                 |
|                                    | 35 10 25 2 - 34 9 26 0  | 93 183.533            | $6.27 \times 10^{-9}$    | 655.1                 |
|                                    | 25 6 20 1 - 25 6 20 0   | 103 300.62            | $4.91 \times 10^{-9}$    | 376.3                 |
|                                    | 7 0 7 0 - 6 1 6 0       | 103 300.759           | $6.84 \times 10^{-8}$    | 79.9                  |
|                                    | 4 2 3 1 - 4 0 4 1       | 103 320.469           | $1.28 \times 10^{-8}$    | 74.8                  |
|                                    | 34 8 26 1 - 34 8 26 0   | 103 381.264           | $9.03 \times 10^{-9}$    | 635.1                 |
|                                    | 34 8 27 1 - 34 8 27 0   | 103 385.983           | $8.98 \times 10^{-9}$    | 635.1                 |
|                                    | 9 2 8 1 - 9 1 9 1       | 103 387.337           | $2.99 \times 10^{-8}$    | 103.7                 |
|                                    | 37 9 28 1 - 37 9 28 0   | 103 403.957           | $2.12 \times 10^{-8}$    | 745.6                 |
| 37 9 29 1 - 37 9 29 0              | 103 404.936             | $2.12 \times 10^{-8}$ | 745.6                    |                       |

Table B.2: continued.

| Species                             | Transition<br>J K L M   | Frequency<br>(MHz) | $A_{ij}$<br>( $s^{-1}$ ) | $E_{up}$<br>(K) |
|-------------------------------------|-------------------------|--------------------|--------------------------|-----------------|
|                                     | 27 5 22 0 - 26 6 20 1   | 103 422.99         | $1.25 \times 10^{-6}$    | 403.0           |
|                                     | 15 2 13 0 - 15 0 15 1   | 103 431.155        | $1.90 \times 10^{-8}$    | 163.3           |
|                                     | 6 2 5 0 - 5 2 4 0       | 103 452.151        | $8.32 \times 10^{-6}$    | 79.2            |
|                                     | 38 11 27 1 - 38 11 27 0 | 103 457.114        | $1.75 \times 10^{-8}$    | 825.6           |
|                                     | 38 11 28 1 - 38 11 28 0 | 103 457.118        | $1.75 \times 10^{-8}$    | 825.6           |
|                                     | 6 2 5 0 - 6 0 6 0       | 103 463.245        | $5.33 \times 10^{-7}$    | 79.2            |
|                                     | 6 0 6 2 - 5 0 5 2       | 103 480.355        | $1.26 \times 10^{-8}$    | 17.5            |
|                                     | 9 1 8 0 - 8 2 7 0       | 103 488.524        | $7.92 \times 10^{-8}$    | 96.5            |
| CH <sub>2</sub> DCH <sub>2</sub> OH | 44 3 41 - 43 6 38       | 90 856.753         | $1.14 \times 10^{-7}$    | 811.0           |
|                                     | 8 2 7 - 8 1 8           | 90 874.001         | $3.63 \times 10^{-6}$    | 33.4            |
| CH <sub>3</sub> CHDOH               | 46 6 40 - 45 9 37       | 90 764.508         | $9.58 \times 10^{-8}$    | 946.6           |
|                                     | 11 3 8 - 11 2 9         | 90 800.322         | $5.71 \times 10^{-6}$    | 64.1            |
|                                     | 13 2 12 - 12 3 9        | 90 973.356         | $8.44 \times 10^{-7}$    | 78.6            |
|                                     | 5 5 1 - 6 4 2           | 91 219.103         | $1.43 \times 10^{-7}$    | 38.3            |
|                                     | 5 5 0 - 6 4 3           | 91 220.883         | $1.43 \times 10^{-7}$    | 38.3            |
|                                     | 15 9 7 - 16 8 8         | 91 235.784         | $5.29 \times 10^{-7}$    | 183.0           |
|                                     | 15 9 6 - 16 8 9         | 91 235.788         | $5.29 \times 10^{-7}$    | 183.0           |
|                                     | 10 7 4 - 11 6 5         | 91 299.292         | $4.07 \times 10^{-7}$    | 96.2            |
|                                     | 10 7 3 - 11 6 6         | 91 299.396         | $4.07 \times 10^{-7}$    | 96.2            |
|                                     | 7 3 4 - 7 2 5           | 103 415.2          | $6.61 \times 10^{-6}$    | 32.5            |
|                                     | 20 2 19 - 19 3 16       | 103 499.655        | $3.16 \times 10^{-7}$    | 174.2           |
|                                     | 11 2 9 - 10 3 8         | 103 508.282        | $2.08 \times 10^{-6}$    | 59.8            |
| CH <sub>3</sub> OCHO                | 27 16 12 4 - 28 15 14 4 | 90 592.278         | $1.03 \times 10^{-7}$    | 580.3           |
|                                     | 23 3 20 0 - 24 2 23 0   | 90 649.201         | $7.44 \times 10^{-9}$    | 173.2           |
|                                     | 33 19 14 2 - 34 18 16 2 | 90 707.602         | $1.06 \times 10^{-7}$    | 570.2           |
|                                     | 33 19 15 1 - 34 18 17 1 | 90 719.908         | $1.06 \times 10^{-7}$    | 570.2           |
|                                     | 33 19 14 0 - 34 18 17 0 | 90 740.574         | $1.06 \times 10^{-7}$    | 570.2           |
|                                     | 33 19 15 0 - 34 18 16 0 | 90 740.574         | $1.06 \times 10^{-7}$    | 570.2           |
|                                     | 9 4 6 1 - 9 3 6 2       | 90 876.84          | $6.31 \times 10^{-8}$    | 37.2            |
|                                     | 17 3 14 5 - 17 2 15 5   | 90 937.614         | $1.13 \times 10^{-6}$    | 286.2           |
|                                     | 27 16 11 5 - 28 15 13 5 | 91 018.326         | $1.04 \times 10^{-7}$    | 580.5           |
|                                     | 19 5 14 5 - 19 4 15 5   | 91 089.478         | $1.38 \times 10^{-6}$    | 316.9           |
|                                     | 36 5 31 3 - 35 7 28 3   | 91 134.07          | $2.89 \times 10^{-8}$    | 603.3           |
|                                     | 26 8 19 3 - 25 9 16 3   | 91 161.894         | $2.21 \times 10^{-7}$    | 437.0           |
|                                     | 26 8 18 5 - 25 9 16 5   | 91 164.314         | $2.14 \times 10^{-7}$    | 437.1           |
|                                     | 36 20 16 5 - 37 19 18 5 | 91 179.846         | $1.14 \times 10^{-7}$    | 845.3           |
|                                     | 34 6 29 0 - 35 4 32 0   | 91 179.968         | $8.61 \times 10^{-9}$    | 377.6           |
|                                     | 34 6 29 0 - 35 3 32 0   | 91 194.313         | $1.29 \times 10^{-8}$    | 377.6           |
|                                     | 9 4 5 0 - 9 3 6 0       | 91 356.766         | $1.03 \times 10^{-6}$    | 37.2            |
|                                     | 9 4 5 2 - 9 3 6 2       | 91 366.495         | $9.71 \times 10^{-7}$    | 37.3            |
|                                     | 14 2 12 2 - 14 2 13 1   | 91 381.738         | $4.08 \times 10^{-7}$    | 67.0            |
|                                     | 10 3 8 1 - 10 1 9 2     | 93 160.968         | $2.82 \times 10^{-7}$    | 38.5            |
|                                     | 12 3 10 3 - 12 2 11 3   | 93 180.635         | $9.90 \times 10^{-7}$    | 239.5           |
|                                     | 10 3 8 0 - 10 1 9 0     | 93 190.933         | $2.83 \times 10^{-7}$    | 38.5            |
|                                     | 43 15 29 4 - 42 16 27 4 | 103 307.836        | $2.85 \times 10^{-7}$    | 893.2           |
|                                     | 32 19 13 2 - 33 18 15 2 | 103 335.016        | $1.47 \times 10^{-7}$    | 550.7           |
|                                     | 32 19 14 1 - 33 18 16 1 | 103 342.834        | $1.47 \times 10^{-7}$    | 550.7           |
|                                     | 25 6 19 5 - 25 5 20 5   | 103 367.418        | $2.23 \times 10^{-6}$    | 405.1           |
|                                     | 32 19 13 0 - 33 18 16 0 | 103 367.795        | $1.47 \times 10^{-7}$    | 550.7           |
|                                     | 32 19 14 0 - 33 18 15 0 | 103 367.795        | $1.47 \times 10^{-7}$    | 550.7           |
|                                     | 24 6 18 0 - 24 5 19 0   | 103 376.842        | $2.21 \times 10^{-6}$    | 203.8           |
|                                     | 24 6 18 2 - 24 5 19 2   | 103 387.2          | $2.21 \times 10^{-6}$    | 203.8           |
|                                     | 36 12 24 5 - 35 13 22 5 | 103 456.449        | $3.03 \times 10^{-7}$    | 675.5           |
|                                     | 8 2 6 2 - 7 2 5 2       | 103 466.572        | $1.52 \times 10^{-5}$    | 24.6            |
|                                     | 25 6 19 3 - 25 5 20 3   | 103 469.71         | $2.28 \times 10^{-6}$    | 405.0           |
|                                     | 8 2 6 0 - 7 2 5 0       | 103 478.663        | $1.52 \times 10^{-5}$    | 24.6            |



Table B.2: continued.

| Species                          | Transition<br>J K L M             | Frequency<br>(MHz)      | $A_{ij}$<br>( $s^{-1}$ ) | $E_{up}$<br>(K)       |
|----------------------------------|-----------------------------------|-------------------------|--------------------------|-----------------------|
| CH <sub>3</sub> OCH <sub>3</sub> | 15 3 12 0 - 14 4 11 0             | 90 889.262              | $1.02 \times 10^{-6}$    | 122.5                 |
|                                  | 15 3 12 1 - 14 4 11 1             | 90 892.26               | $1.02 \times 10^{-6}$    | 122.5                 |
|                                  | 15 3 12 5 - 14 4 11 5             | 90 895.187              | $1.02 \times 10^{-6}$    | 122.5                 |
|                                  | 15 3 12 3 - 14 4 11 3             | 90 895.33               | $1.02 \times 10^{-6}$    | 122.5                 |
|                                  | 6 0 6 0 - 5 1 5 0                 | 90 937.508              | $3.63 \times 10^{-6}$    | 19.0                  |
|                                  | 6 0 6 1 - 5 1 5 1                 | 90 938.107              | $3.63 \times 10^{-6}$    | 19.0                  |
|                                  | 6 0 6 5 - 5 1 5 5                 | 90 938.705              | $3.63 \times 10^{-6}$    | 19.0                  |
|                                  | 6 0 6 3 - 5 1 5 3                 | 90 938.707              | $3.63 \times 10^{-6}$    | 19.0                  |
|                                  | 5 3 2 3 - 6 4 2 3                 | 91 164.996              | $1.15 \times 10^{-7}$    | 36.1                  |
|                                  | 5 3 2 1 - 6 4 3 1                 | 91 175.203              | $1.44 \times 10^{-7}$    | 36.1                  |
|                                  | 5 3 2 5 - 6 4 3 5                 | 91 176.676              | $3.45 \times 10^{-7}$    | 36.1                  |
|                                  | 5 3 2 0 - 6 4 3 0                 | 91 184.531              | $3.46 \times 10^{-7}$    | 36.1                  |
|                                  | 5 3 2 3 - 6 4 3 3                 | 91 185.031              | $2.31 \times 10^{-7}$    | 36.2                  |
|                                  | 5 3 2 1 - 6 4 2 1                 | 91 185.221              | $2.02 \times 10^{-7}$    | 36.1                  |
|                                  | 5 3 3 3 - 6 4 2 3                 | 91 223.214              | $2.31 \times 10^{-7}$    | 36.1                  |
|                                  | 5 3 3 1 - 6 4 3 1                 | 91 230.878              | $2.02 \times 10^{-7}$    | 36.1                  |
|                                  | 5 3 3 5 - 6 4 2 5                 | 91 231.569              | $3.46 \times 10^{-7}$    | 36.1                  |
|                                  | 5 3 3 0 - 6 4 2 0                 | 91 239.423              | $3.47 \times 10^{-7}$    | 36.1                  |
|                                  | 5 3 3 1 - 6 4 2 1                 | 91 240.896              | $1.44 \times 10^{-7}$    | 36.1                  |
|                                  | 5 3 3 3 - 6 4 3 3                 | 91 243.249              | $1.16 \times 10^{-7}$    | 36.2                  |
|                                  | 9 0 9 3 - 10 3 8 3                | 91 345.408              | $2.47 \times 10^{-8}$    | 53.6                  |
|                                  | 9 0 9 5 - 10 3 8 5                | 91 345.55               | $2.47 \times 10^{-8}$    | 53.6                  |
|                                  | 9 0 9 1 - 10 3 8 1                | 91 351.871              | $2.51 \times 10^{-8}$    | 53.6                  |
|                                  | 9 0 9 0 - 10 3 8 0                | 91 358.263              | $2.53 \times 10^{-8}$    | 53.6                  |
|                                  | 32 12 20 3 - 33 13 20 3           | 103 489.911             | $1.08 \times 10^{-6}$    | 717.6                 |
|                                  | 32 12 21 1 - 33 13 21 1           | 103 489.975             | $1.08 \times 10^{-6}$    | 717.6                 |
|                                  | 32 12 20 0 - 33 13 21 0           | 103 490.039             | $1.08 \times 10^{-6}$    | 717.6                 |
|                                  | 32 12 21 0 - 33 13 20 0           | 103 490.039             | $1.08 \times 10^{-6}$    | 717.6                 |
|                                  | 32 12 20 5 - 33 13 21 5           | 103 490.157             | $1.08 \times 10^{-6}$    | 717.6                 |
|                                  | 32 12 21 5 - 33 13 20 5           | 103 490.157             | $1.08 \times 10^{-6}$    | 717.6                 |
|                                  | 32 12 20 1 - 33 13 20 1           | 103 490.221             | $1.08 \times 10^{-6}$    | 717.6                 |
|                                  | 32 12 21 3 - 33 13 21 3           | 103 490.403             | $1.08 \times 10^{-6}$    | 717.6                 |
|                                  | CH <sub>3</sub> COCH <sub>3</sub> | 41 27 14 0 - 41 26 15 0 | 90 595.197               | $2.62 \times 10^{-5}$ |
| 20 17 3 2 - 20 16 4 2            |                                   | 90 598.617              | $1.28 \times 10^{-5}$    | 186.7                 |
| 20 17 4 2 - 20 16 5 2            |                                   | 90 636.946              | $1.29 \times 10^{-5}$    | 186.7                 |
| 20 17 3 3 - 20 16 4 3            |                                   | 90 688.355              | $1.29 \times 10^{-5}$    | 186.8                 |
| 13 3 10 1 - 13 2 11 1            |                                   | 90 690.157              | $9.47 \times 10^{-6}$    | 59.9                  |
| 13 4 10 1 - 13 3 11 1            |                                   | 90 690.212              | $9.47 \times 10^{-6}$    | 59.9                  |
| 9 7 2 3 - 8 8 0 3                |                                   | 90 808.887              | $4.05 \times 10^{-7}$    | 38.5                  |
| 27 19 8 1 - 27 18 10 1           |                                   | 90 812.649              | $6.42 \times 10^{-7}$    | 315.8                 |
| 12 2 10 2 - 12 1 11 2            |                                   | 90 841.133              | $7.02 \times 10^{-6}$    | 48.5                  |
| 12 3 10 2 - 12 2 11 2            |                                   | 90 841.14               | $7.02 \times 10^{-6}$    | 48.5                  |
| 12 2 10 3 - 12 1 11 3            |                                   | 90 841.209              | $7.02 \times 10^{-6}$    | 48.5                  |
| 12 3 10 3 - 12 2 11 3            |                                   | 90 841.217              | $7.02 \times 10^{-6}$    | 48.5                  |
| 13 3 10 0 - 13 2 11 0            |                                   | 90 842.133              | $9.52 \times 10^{-6}$    | 59.8                  |
| 13 4 10 0 - 13 3 11 0            |                                   | 90 842.19               | $9.53 \times 10^{-6}$    | 59.8                  |
| 20 17 4 1 - 20 16 5 1            |                                   | 90 855.834              | $1.29 \times 10^{-5}$    | 186.7                 |
| 13 6 7 1 - 12 9 4 1              |                                   | 90 879.456              | $1.57 \times 10^{-7}$    | 70.3                  |
| 7 3 5 3 - 6 2 4 3                |                                   | 90 884.785              | $2.10 \times 10^{-5}$    | 19.7                  |
| 7 3 5 2 - 6 2 4 2                |                                   | 90 889.558              | $2.10 \times 10^{-5}$    | 19.7                  |
| 20 17 3 1 - 20 16 4 1            |                                   | 90 927.486              | $1.29 \times 10^{-5}$    | 186.8                 |
| 26 19 8 3 - 26 18 9 3            |                                   | 90 930.919              | $1.63 \times 10^{-5}$    | 296.2                 |
| 7 3 5 1 - 6 2 4 1                |                                   | 90 936.196              | $2.10 \times 10^{-5}$    | 19.6                  |
| 23 12 11 2 - 23 11 12 2          |                                   | 90 947.328              | $2.04 \times 10^{-5}$    | 218.4                 |
| 23 12 11 3 - 23 11 12 3          |                                   | 90 950.792              | $2.04 \times 10^{-5}$    | 218.4                 |
| 27 19 8 3 - 27 18 10 3           |                                   | 90 959.492              | $1.83 \times 10^{-6}$    | 315.8                 |

Table B.2: continued.

| Species              | Transition<br>J K L M       | Frequency<br>(MHz) | $A_{ij}$<br>( $s^{-1}$ ) | $E_{up}$<br>(K) |
|----------------------|-----------------------------|--------------------|--------------------------|-----------------|
|                      | 23 12 11 1 - 23 11 12 1     | 90 964.992         | $2.04 \times 10^{-5}$    | 218.4           |
|                      | 9 7 3 3 - 8 8 1 3           | 90 965.369         | $4.04 \times 10^{-7}$    | 38.3            |
|                      | 41 27 14 1 - 41 26 15 1     | 90 972.394         | $2.64 \times 10^{-5}$    | 708.7           |
|                      | 22 8 14 1 - 21 11 11 1      | 90 977.509         | $7.34 \times 10^{-8}$    | 183.5           |
|                      | 23 12 11 0 - 23 11 12 0     | 90 981.426         | $2.04 \times 10^{-5}$    | 218.4           |
|                      | 7 3 5 0 - 6 2 4 0           | 90 985.117         | $2.10 \times 10^{-5}$    | 19.5            |
|                      | 12 2 10 1 - 12 1 11 1       | 91 005.085         | $7.06 \times 10^{-6}$    | 48.4            |
|                      | 12 3 10 1 - 12 2 11 1       | 91 005.092         | $7.06 \times 10^{-6}$    | 48.4            |
|                      | 9 7 2 1 - 8 8 0 1           | 91 057.153         | $3.53 \times 10^{-7}$    | 38.4            |
|                      | 11 1 10 2 - 11 0 11 2       | 91 077.508         | $3.96 \times 10^{-6}$    | 37.8            |
|                      | 11 2 10 2 - 11 1 11 2       | 91 077.509         | $3.96 \times 10^{-6}$    | 37.8            |
|                      | 11 1 10 3 - 11 0 11 3       | 91 077.598         | $3.96 \times 10^{-6}$    | 37.8            |
|                      | 11 2 10 3 - 11 1 11 3       | 91 077.598         | $3.96 \times 10^{-6}$    | 37.8            |
|                      | 23 18 5 2 - 23 17 6 2       | 91 131.97          | $1.70 \times 10^{-5}$    | 238.0           |
|                      | 22 9 14 1 - 21 10 11 1      | 91 132.382         | $7.38 \times 10^{-8}$    | 183.5           |
|                      | 20 17 3 0 - 20 16 4 0       | 91 146.721         | $1.30 \times 10^{-5}$    | 186.7           |
|                      | 12 2 10 0 - 12 1 11 0       | 91 168.75          | $7.11 \times 10^{-6}$    | 48.3            |
|                      | 12 3 10 0 - 12 2 11 0       | 91 168.757         | $7.11 \times 10^{-6}$    | 48.3            |
|                      | 20 17 4 0 - 20 16 5 0       | 91 183.074         | $1.30 \times 10^{-5}$    | 186.7           |
|                      | 41 25 16 2 - 41 24 17 2     | 91 202.244         | $2.72 \times 10^{-5}$    | 700.6           |
|                      | 41 25 16 3 - 41 24 17 3     | 91 205.905         | $2.72 \times 10^{-5}$    | 700.6           |
|                      | 11 1 10 1 - 11 0 11 1       | 91 252.28          | $3.99 \times 10^{-6}$    | 37.7            |
|                      | 11 2 10 1 - 11 1 11 1       | 91 252.281         | $3.99 \times 10^{-6}$    | 37.7            |
|                      | 41 27 14 2 - 41 26 15 2     | 91 294.888         | $2.67 \times 10^{-5}$    | 708.7           |
|                      | 23 18 6 3 - 23 17 7 3       | 91 296.205         | $1.70 \times 10^{-5}$    | 237.9           |
|                      | 41 25 16 1 - 41 24 17 1     | 91 318.968         | $2.73 \times 10^{-5}$    | 700.7           |
|                      | 41 27 14 3 - 41 26 15 3     | 91 393.556         | $2.66 \times 10^{-5}$    | 708.7           |
|                      | 9 6 4 3 - 8 7 1 3           | 93 175.842         | $5.69 \times 10^{-7}$    | 36.6            |
|                      | 25 19 7 1 - 25 18 7 1       | 93 183.007         | $1.96 \times 10^{-6}$    | 277.6           |
|                      | 8 5 3 1 - 8 2 6 1           | 103 297.162        | $1.37 \times 10^{-7}$    | 29.4            |
|                      | 31 22 10 2 - 31 21 11 2     | 103 298.616        | $3.10 \times 10^{-5}$    | 415.4           |
|                      | 24 10 15 1 - 23 11 12 1     | 103 309.761        | $1.14 \times 10^{-7}$    | 219.0           |
|                      | 31 22 10 1 - 31 21 11 1     | 103 352.24         | $3.07 \times 10^{-5}$    | 415.4           |
|                      | 42 28 14 1 - 42 27 15 1     | 103 365.841        | $3.62 \times 10^{-5}$    | 745.1           |
|                      | 31 22 10 0 - 31 21 11 0     | 103 425.624        | $3.11 \times 10^{-5}$    | 415.5           |
| CH <sub>3</sub> COOH | 9 5 4 0 0 - 8 7 1 0 0       | 90 619.38          | $1.29 \times 10^{-8}$    | 40.6            |
|                      | 21 13 9 0 2 - 20 16 4 0 1   | 90 638.822         | $4.29 \times 10^{-9}$    | 207.8           |
|                      | 22 8 14 0 1 - 21 10 11 0 2  | 90 670.076         | $4.28 \times 10^{-9}$    | 203.4           |
|                      | 22 9 14 0 1 - 21 10 11 0 2  | 90 670.227         | $1.80 \times 10^{-8}$    | 203.4           |
|                      | 23 17 6 0 1 - 23 16 7 0 2   | 90 689.582         | $4.84 \times 10^{-6}$    | 260.4           |
|                      | 35 13 23 0 2 - 34 15 20 0 1 | 90 716.134         | $2.96 \times 10^{-9}$    | 496.3           |
|                      | 35 12 23 0 2 - 34 15 20 0 1 | 90 716.134         | $1.12 \times 10^{-8}$    | 496.3           |
|                      | 35 12 23 0 2 - 34 14 20 0 1 | 90 716.15          | $2.96 \times 10^{-9}$    | 496.3           |
|                      | 35 13 23 0 2 - 34 14 20 0 1 | 90 716.15          | $1.12 \times 10^{-8}$    | 496.3           |
|                      | 8 6 2 0 0 - 8 4 5 0 0       | 90 727.049         | $2.18 \times 10^{-8}$    | 34.4            |
|                      | 6 3 4 0 1 - 5 2 3 0 2       | 90 757.201         | $4.46 \times 10^{-6}$    | 17.0            |
|                      | 13 7 7 0 0 - 12 9 3 0 0     | 90 762.796         | $2.50 \times 10^{-9}$    | 78.4            |
|                      | 9 3 6 0 0 - 8 4 4 0 0       | 90 771.09          | $2.25 \times 10^{-9}$    | 36.3            |
|                      | 36 26 10 0 0 - 35 29 6 0 0  | 90 852.622         | $1.11 \times 10^{-9}$    | 623.9           |
|                      | 27 19 8 0 1 - 27 18 9 0 2   | 90 859.346         | $5.46 \times 10^{-6}$    | 351.7           |
|                      | 10 8 3 0 0 - 10 5 5 0 0     | 90 898.339         | $1.21 \times 10^{-7}$    | 52.9            |
|                      | 8 6 2 0 0 - 7 7 0 0 0       | 90 901.78          | $1.30 \times 10^{-7}$    | 34.4            |
|                      | 25 13 13 0 0 - 24 16 8 0 0  | 90 917.361         | $3.12 \times 10^{-9}$    | 280.1           |
|                      | 22 14 9 0 2 - 21 17 4 0 1   | 90 947.862         | $3.54 \times 10^{-9}$    | 229.2           |
|                      | 35 19 16 0 0 - 34 24 11 0 0 | 90 949.971         | $1.58 \times 10^{-9}$    | 558.0           |
|                      | 15 9 6 0 0 - 14 12 2 0 0    | 90 983.691         | $3.65 \times 10^{-9}$    | 108.9           |

Table B.2: continued.

| Species | Transition<br>J K L M       | Frequency<br>(MHz) | $A_{ij}$<br>( $s^{-1}$ ) | $E_{up}$<br>(K) |
|---------|-----------------------------|--------------------|--------------------------|-----------------|
|         | 44 28 16 0 0 - 44 27 17 0 0 | 90 987.155         | $7.54 \times 10^{-6}$    | 901.4           |
|         | 4 3 1 0 2 - 3 2 2 0 1       | 91 024.622         | $1.97 \times 10^{-6}$    | 9.4             |
|         | 7 5 2 0 0 - 7 3 5 0 0       | 91 062.482         | $1.18 \times 10^{-8}$    | 26.6            |
|         | 8 6 2 0 0 - 8 3 5 0 0       | 91 071.232         | $1.01 \times 10^{-7}$    | 34.4            |
|         | 12 8 5 0 0 - 11 10 2 0 0    | 91 077.987         | $2.76 \times 10^{-9}$    | 71.2            |
|         | 23 17 7 0 0 - 23 16 8 0 0   | 91 088.715         | $4.68 \times 10^{-6}$    | 259.9           |
|         | 38 25 13 0 2 - 38 24 14 0 1 | 91 102.138         | $6.82 \times 10^{-6}$    | 678.6           |
|         | 16 7 9 0 0 - 16 7 10 0 0    | 91 104.88          | $7.50 \times 10^{-7}$    | 115.2           |
|         | 16 7 9 0 0 - 16 6 10 0 0    | 91 109.457         | $4.22 \times 10^{-6}$    | 115.2           |
|         | 33 20 13 0 2 - 33 19 14 0 1 | 91 118.246         | $6.41 \times 10^{-6}$    | 507.8           |
|         | 22 12 10 0 1 - 22 12 11 0 2 | 91 139.444         | $8.11 \times 10^{-7}$    | 224.9           |
|         | 7 5 2 0 0 - 7 2 5 0 0       | 91 145.635         | $5.62 \times 10^{-8}$    | 26.6            |
|         | 9 7 2 0 1 - 9 5 5 0 2       | 91 159.53          | $5.66 \times 10^{-8}$    | 42.9            |
|         | 16 8 9 0 0 - 16 7 10 0 0    | 91 190.673         | $4.23 \times 10^{-6}$    | 115.2           |
|         | 16 8 9 0 0 - 16 6 10 0 0    | 91 195.251         | $7.52 \times 10^{-7}$    | 115.2           |
|         | 8 4 4 0 0 - 7 6 2 0 0       | 91 196.807         | $1.85 \times 10^{-8}$    | 32.0            |
|         | 27 14 14 0 0 - 26 17 9 0 0  | 91 250.365         | $2.62 \times 10^{-9}$    | 325.9           |
|         | 6 3 3 0 0 - 5 4 2 0 0       | 91 269.118         | $1.58 \times 10^{-6}$    | 18.9            |
|         | 21 16 6 0 1 - 21 15 7 0 2   | 91 299.04          | $4.57 \times 10^{-6}$    | 220.0           |
|         | 25 18 7 0 2 - 25 17 8 0 1   | 91 334.072         | $5.25 \times 10^{-6}$    | 304.3           |
|         | 23 15 9 0 0 - 23 13 10 0 0  | 91 339.865         | $5.76 \times 10^{-7}$    | 251.5           |
|         | 30 8 23 0 2 - 31 5 26 0 1   | 91 340.082         | $1.66 \times 10^{-9}$    | 333.7           |
|         | 30 7 23 0 2 - 31 6 26 0 1   | 91 340.082         | $1.66 \times 10^{-9}$    | 333.7           |
|         | 17 12 5 0 0 - 17 10 7 0 0   | 91 354.78          | $8.80 \times 10^{-8}$    | 142.6           |
|         | 16 7 9 0 2 - 16 7 10 0 1    | 91 372.165         | $7.96 \times 10^{-7}$    | 115.0           |
|         | 16 7 9 0 2 - 16 6 10 0 1    | 91 380.62          | $4.25 \times 10^{-6}$    | 115.0           |
|         | 21 14 8 0 1 - 21 12 9 0 2   | 91 402.908         | $4.92 \times 10^{-7}$    | 211.6           |
|         | 5 3 3 0 0 - 4 1 3 0 0       | 103 295.419        | $3.09 \times 10^{-9}$    | 13.2            |
|         | 37 13 24 0 1 - 36 16 21 0 2 | 103 296.257        | $1.76 \times 10^{-8}$    | 557.0           |
|         | 37 14 24 0 1 - 36 16 21 0 2 | 103 296.257        | $4.57 \times 10^{-9}$    | 557.0           |
|         | 37 14 24 0 1 - 36 15 21 0 2 | 103 296.268        | $1.76 \times 10^{-8}$    | 557.0           |
|         | 37 13 24 0 1 - 36 15 21 0 2 | 103 296.268        | $4.57 \times 10^{-9}$    | 557.0           |
|         | 46 30 16 0 0 - 46 29 17 0 0 | 103 322.329        | $1.03 \times 10^{-5}$    | 987.8           |
|         | 39 26 13 0 2 - 39 25 14 0 1 | 103 324.61         | $9.26 \times 10^{-6}$    | 716.2           |
|         | 17 13 4 0 0 - 16 15 1 0 0   | 103 347.172        | $1.82 \times 10^{-9}$    | 145.9           |
|         | 25 15 11 0 2 - 25 13 12 0 1 | 103 356.352        | $1.15 \times 10^{-6}$    | 290.6           |
|         | 14 4 10 0 0 - 14 4 11 0 0   | 103 356.454        | $8.11 \times 10^{-7}$    | 80.3            |
|         | 14 4 10 0 0 - 14 3 11 0 0   | 103 356.459        | $4.22 \times 10^{-6}$    | 80.3            |
|         | 14 5 10 0 0 - 14 4 11 0 0   | 103 356.671        | $4.22 \times 10^{-6}$    | 80.3            |
|         | 14 5 10 0 0 - 14 3 11 0 0   | 103 356.676        | $8.11 \times 10^{-7}$    | 80.3            |
|         | 23 18 6 0 0 - 23 17 7 0 0   | 103 357.115        | $6.18 \times 10^{-6}$    | 264.9           |
|         | 37 25 12 0 0 - 37 24 13 0 0 | 103 369.818        | $8.93 \times 10^{-6}$    | 647.3           |
|         | 24 9 15 0 2 - 23 11 12 0 1  | 103 397.728        | $6.75 \times 10^{-9}$    | 242.8           |
|         | 24 10 15 0 2 - 23 11 12 0 1 | 103 397.836        | $2.84 \times 10^{-8}$    | 242.8           |
|         | 30 20 11 0 0 - 30 19 12 0 0 | 103 402.047        | $8.44 \times 10^{-6}$    | 426.4           |
|         | 38 10 29 0 0 - 39 7 32 0 0  | 103 406.702        | $2.41 \times 10^{-9}$    | 531.8           |
|         | 38 9 29 0 0 - 39 8 32 0 0   | 103 406.702        | $2.41 \times 10^{-9}$    | 531.8           |
|         | 4 2 2 0 0 - 3 1 3 0 0       | 103 412.258        | $5.21 \times 10^{-7}$    | 9.3             |
|         | 18 14 5 0 0 - 17 16 2 0 0   | 103 452.707        | $1.38 \times 10^{-9}$    | 163.5           |
|         | 6 4 2 0 1 - 5 4 1 0 2       | 103 468.297        | $2.68 \times 10^{-6}$    | 19.3            |
|         | 15 5 10 0 1 - 15 5 11 0 2   | 103 469.421        | $9.90 \times 10^{-7}$    | 94.9            |
|         | 15 5 10 0 1 - 15 4 11 0 2   | 103 469.491        | $4.83 \times 10^{-6}$    | 94.9            |
|         | 15 6 10 0 1 - 15 5 11 0 2   | 103 471.5          | $4.83 \times 10^{-6}$    | 94.9            |
|         | 15 6 10 0 1 - 15 4 11 0 2   | 103 471.57         | $9.90 \times 10^{-7}$    | 94.9            |
|         | 34 24 11 0 0 - 33 27 6 0 0  | 103 481.533        | $2.07 \times 10^{-9}$    | 553.7           |
|         | 4 2 2 0 0 - 3 0 3 0 0       | 103 486.332        | $1.19 \times 10^{-7}$    | 9.3             |

Table B.2: continued.

| Species                             | Transition<br>J K L M | Frequency<br>(MHz)    | $A_{ij}$<br>( $s^{-1}$ ) | $E_{up}$<br>(K) |
|-------------------------------------|-----------------------|-----------------------|--------------------------|-----------------|
| CH <sub>2</sub> OHCHO               | 11 2 10 - 11 1 11     | 90 591.344            | $5.85 \times 10^{-6}$    | 38.2            |
|                                     | 4 2 2 - 3 1 3         | 90 785.464            | $6.54 \times 10^{-6}$    | 8.0             |
|                                     | 11 4 8 - 11 3 9       | 90 922.214            | $1.24 \times 10^{-5}$    | 46.5            |
|                                     | 32 11 22 - 31 12 19   | 90 940.226            | $2.43 \times 10^{-6}$    | 368.0           |
|                                     | 32 11 21 - 31 12 20   | 90 977.093            | $2.43 \times 10^{-6}$    | 368.0           |
|                                     | 43 16 28 - 42 17 25   | 91 277.849            | $2.30 \times 10^{-6}$    | 682.0           |
|                                     | 43 16 27 - 42 17 26   | 91 277.921            | $2.30 \times 10^{-6}$    | 682.0           |
|                                     | 10 0 10 - 9 1 9       | 103 391.285           | $2.79 \times 10^{-5}$    | 28.3            |
| 15 4 12 - 15 3 13                   | 103 461.311           | $1.78 \times 10^{-5}$ | 76.8                     |                 |
| <sup>13</sup> CH <sub>2</sub> OHCHO | 49 19 31 - 48 20 28   | 90 623.698            | $2.17 \times 10^{-6}$    | 891.0           |
|                                     | 49 19 30 - 48 20 29   | 90 623.7              | $2.17 \times 10^{-6}$    | 891.0           |
|                                     | 23 5 18 - 23 4 19     | 90 629.152            | $1.69 \times 10^{-5}$    | 171.7           |
|                                     | 24 6 18 - 24 5 19     | 90 745.683            | $1.83 \times 10^{-5}$    | 190.0           |
|                                     | 33 20 13 - 34 19 16   | 90 765.157            | $1.15 \times 10^{-6}$    | 546.9           |
|                                     | 33 20 14 - 34 19 15   | 90 765.157            | $1.15 \times 10^{-6}$    | 546.9           |
|                                     | 6 4 3 - 7 1 6         | 90 791.284            | $1.47 \times 10^{-8}$    | 21.1            |
|                                     | 23 3 20 - 24 2 23     | 90 833.934            | $7.95 \times 10^{-8}$    | 161.2           |
|                                     | 12 3 10 - 12 1 11     | 91 019.113            | $9.70 \times 10^{-9}$    | 48.3            |
|                                     | 17 3 14 - 17 2 15     | 91 123.479            | $1.24 \times 10^{-5}$    | 93.1            |
|                                     | 18 13 5 - 19 12 8     | 91 151.742            | $7.59 \times 10^{-7}$    | 194.7           |
|                                     | 18 13 6 - 19 12 7     | 91 151.742            | $7.59 \times 10^{-7}$    | 194.7           |
|                                     | 25 6 19 - 25 5 20     | 91 236.931            | $1.88 \times 10^{-5}$    | 204.6           |
|                                     | 12 4 9 - 12 3 10      | 91 277.72             | $1.26 \times 10^{-5}$    | 52.7            |
|                                     | 9 7 3 - 8 7 2         | 103 285.896           | $1.65 \times 10^{-7}$    | 53.9            |
|                                     | 9 7 2 - 8 7 1         | 103 285.9             | $1.65 \times 10^{-7}$    | 53.9            |
|                                     | 37 13 25 - 36 14 22   | 103 343.428           | $3.52 \times 10^{-6}$    | 489.6           |
|                                     | 37 13 24 - 36 14 23   | 103 349.948           | $3.52 \times 10^{-6}$    | 489.6           |
|                                     | 9 6 4 - 8 6 3         | 103 420.473           | $2.33 \times 10^{-7}$    | 46.2            |
|                                     | 9 6 3 - 8 6 2         | 103 420.752           | $2.33 \times 10^{-7}$    | 46.2            |
| 26 8 18 - 25 9 17                   | 103 459.303           | $3.85 \times 10^{-6}$ | 233.1                    |                 |
| 52 8 44 - 53 7 47                   | 103 468.404           | $2.66 \times 10^{-7}$ | 815.0                    |                 |
| CHDOHCHO                            | 8 5 4 - 7 5 3         | 90 593.937            | $1.71 \times 10^{-7}$    | 33.1            |
|                                     | 22 16 6 - 23 15 9     | 90 597.888            | $6.78 \times 10^{-7}$    | 276.4           |
|                                     | 22 16 7 - 23 15 8     | 90 597.888            | $6.78 \times 10^{-7}$    | 276.4           |
|                                     | 8 5 3 - 7 5 2         | 90 599.345            | $1.71 \times 10^{-7}$    | 33.1            |
|                                     | 3 3 0 - 2 2 1         | 90 655.047            | $1.65 \times 10^{-5}$    | 8.2             |
|                                     | 8 3 6 - 7 3 5         | 90 678.44             | $2.41 \times 10^{-7}$    | 24.5            |
|                                     | 46 8 39 - 47 5 42     | 90 679.401            | $1.48 \times 10^{-7}$    | 625.6           |
|                                     | 17 3 14 - 17 2 15     | 90 722.053            | $1.16 \times 10^{-5}$    | 91.2            |
|                                     | 20 15 5 - 21 14 8     | 90 728.937            | $6.15 \times 10^{-7}$    | 236.2           |
|                                     | 20 15 6 - 21 14 7     | 90 728.937            | $6.15 \times 10^{-7}$    | 236.2           |
|                                     | 23 5 18 - 23 4 19     | 90 751.425            | $1.59 \times 10^{-5}$    | 168.3           |
|                                     | 9 0 9 - 8 1 8         | 90 833.314            | $1.85 \times 10^{-5}$    | 22.7            |
|                                     | 18 14 4 - 19 13 7     | 90 851.935            | $5.40 \times 10^{-7}$    | 199.3           |
|                                     | 18 14 5 - 19 13 6     | 90 851.935            | $5.40 \times 10^{-7}$    | 199.3           |
|                                     | 8 4 5 - 7 4 4         | 90 856.595            | $2.12 \times 10^{-7}$    | 28.3            |
|                                     | 16 13 3 - 17 12 6     | 90 964.082            | $4.53 \times 10^{-7}$    | 165.7           |
|                                     | 16 13 4 - 17 12 5     | 90 964.082            | $4.53 \times 10^{-7}$    | 165.7           |
|                                     | 20 4 16 - 20 3 17     | 91 001.685            | $1.40 \times 10^{-5}$    | 126.9           |
|                                     | 8 4 4 - 7 4 3         | 91 021.872            | $2.13 \times 10^{-7}$    | 28.3            |
|                                     | 14 12 2 - 15 11 5     | 91 062.071            | $3.52 \times 10^{-7}$    | 135.3           |
|                                     | 14 12 3 - 15 11 4     | 91 062.071            | $3.52 \times 10^{-7}$    | 135.3           |
|                                     | 12 11 1 - 13 10 4     | 91 141.943            | $2.36 \times 10^{-7}$    | 108.1           |
|                                     | 12 11 2 - 13 10 3     | 91 141.943            | $2.36 \times 10^{-7}$    | 108.1           |
|                                     | 24 3 21 - 25 2 24     | 91 154.596            | $6.48 \times 10^{-8}$    | 170.4           |
|                                     | 10 10 1 - 11 9 2      | 91 198.912            | $1.11 \times 10^{-7}$    | 84.2            |

Table B.2: continued.

| Species                               | Transition<br>J K L M   | Frequency<br>(MHz) | $A_{ij}$<br>( $s^{-1}$ ) | $E_{up}$<br>(K) |
|---------------------------------------|-------------------------|--------------------|--------------------------|-----------------|
|                                       | 10 10 0 - 11 9 3        | 91 198.912         | $1.11 \times 10^{-7}$    | 84.2            |
|                                       | 9 1 9 - 8 1 8           | 91 353.121         | $2.83 \times 10^{-7}$    | 22.7            |
|                                       | 52 8 44 - 53 7 47       | 93 165.385         | $1.71 \times 10^{-7}$    | 797.6           |
| aGg-(CH <sub>2</sub> OH) <sub>2</sub> | 8 1 7 1 - 7 1 6 0       | 90 593.579         | $1.61 \times 10^{-5}$    | 19.1            |
|                                       | 35 8 28 0 - 35 7 28 1   | 90 635.988         | $3.82 \times 10^{-7}$    | 343.2           |
|                                       | 20 1 19 0 - 19 2 17 1   | 90 642.19          | $6.48 \times 10^{-8}$    | 101.7           |
|                                       | 14 5 10 1 - 14 4 11 1   | 90 662.384         | $2.41 \times 10^{-6}$    | 64.3            |
|                                       | 32 11 22 0 - 31 12 20 1 | 90 674.452         | $1.02 \times 10^{-7}$    | 319.4           |
|                                       | 18 3 16 0 - 17 4 14 1   | 90 675.102         | $5.45 \times 10^{-8}$    | 88.0            |
|                                       | 32 11 21 0 - 31 12 19 1 | 90 675.776         | $1.02 \times 10^{-7}$    | 319.4           |
|                                       | 35 23 12 1 - 36 22 15 1 | 90 680.757         | $1.66 \times 10^{-7}$    | 569.3           |
|                                       | 35 23 13 1 - 36 22 14 1 | 90 680.757         | $1.66 \times 10^{-7}$    | 569.3           |
|                                       | 11 5 6 0 - 11 4 7 0     | 90 683.206         | $1.88 \times 10^{-6}$    | 44.8            |
|                                       | 11 5 6 1 - 11 4 7 1     | 90 686.174         | $1.97 \times 10^{-6}$    | 45.1            |
|                                       | 33 22 11 0 - 34 21 14 0 | 90 701.431         | $1.30 \times 10^{-7}$    | 513.0           |
|                                       | 33 22 12 0 - 34 21 13 0 | 90 701.431         | $1.30 \times 10^{-7}$    | 513.0           |
|                                       | 26 4 22 0 - 26 4 23 1   | 90 726.496         | $8.82 \times 10^{-7}$    | 184.8           |
|                                       | 14 5 10 0 - 14 4 11 0   | 90 731.469         | $1.99 \times 10^{-6}$    | 64.0            |
|                                       | 15 5 11 0 - 15 4 12 0   | 90 752.358         | $2.03 \times 10^{-6}$    | 71.4            |
|                                       | 53 10 43 0 - 53 10 44 1 | 90 785.844         | $7.06 \times 10^{-7}$    | 762.7           |
|                                       | 16 3 14 1 - 16 1 15 0   | 90 802.123         | $6.80 \times 10^{-7}$    | 71.5            |
|                                       | 33 22 11 1 - 34 21 14 1 | 90 839.672         | $1.60 \times 10^{-7}$    | 513.4           |
|                                       | 33 22 12 1 - 34 21 13 1 | 90 839.672         | $1.60 \times 10^{-7}$    | 513.4           |
|                                       | 13 5 9 1 - 13 4 10 1    | 90 852.643         | $2.23 \times 10^{-6}$    | 57.4            |
|                                       | 13 5 9 0 - 13 4 10 0    | 90 857.67          | $1.95 \times 10^{-6}$    | 57.1            |
|                                       | 31 21 10 0 - 32 20 13 0 | 90 864.536         | $1.26 \times 10^{-7}$    | 460.0           |
|                                       | 31 21 11 0 - 32 20 12 0 | 90 864.536         | $1.26 \times 10^{-7}$    | 460.0           |
|                                       | 15 4 11 1 - 15 3 13 0   | 90 866.003         | $2.69 \times 10^{-7}$    | 67.7            |
|                                       | 20 5 16 0 - 19 6 14 1   | 90 918.748         | $1.89 \times 10^{-7}$    | 116.1           |
|                                       | 30 10 21 0 - 29 11 19 1 | 90 926.845         | $1.06 \times 10^{-7}$    | 278.1           |
|                                       | 30 10 20 0 - 29 11 18 1 | 90 933.622         | $1.05 \times 10^{-7}$    | 278.1           |
|                                       | 19 4 16 1 - 19 3 17 1   | 90 968.215         | $1.86 \times 10^{-6}$    | 101.9           |
|                                       | 16 5 12 0 - 16 4 13 0   | 90 992.142         | $2.09 \times 10^{-6}$    | 79.4            |
|                                       | 58 11 47 0 - 58 11 48 1 | 90 996.168         | $6.94 \times 10^{-7}$    | 911.4           |
|                                       | 31 21 10 1 - 32 20 13 1 | 90 996.852         | $1.54 \times 10^{-7}$    | 460.4           |
|                                       | 31 21 11 1 - 32 20 12 1 | 90 996.852         | $1.54 \times 10^{-7}$    | 460.4           |
|                                       | 17 4 13 0 - 16 5 11 1   | 91 008.128         | $2.61 \times 10^{-7}$    | 84.1            |
|                                       | 29 20 9 0 - 30 19 12 0  | 91 025.255         | $1.20 \times 10^{-7}$    | 410.0           |
|                                       | 29 20 10 0 - 30 19 11 0 | 91 025.255         | $1.20 \times 10^{-7}$    | 410.0           |
|                                       | 39 15 25 1 - 38 16 23 0 | 91 041.27          | $8.54 \times 10^{-8}$    | 494.3           |
|                                       | 12 5 8 0 - 12 4 9 0     | 91 067.16          | $1.92 \times 10^{-6}$    | 50.7            |
|                                       | 12 5 8 1 - 12 4 9 1     | 91 076.809         | $2.13 \times 10^{-6}$    | 51.0            |
|                                       | 25 4 21 0 - 25 3 22 0   | 91 106.286         | $2.05 \times 10^{-6}$    | 171.7           |
|                                       | 31 7 24 1 - 31 6 25 1   | 91 112.101         | $3.06 \times 10^{-6}$    | 270.7           |
|                                       | 29 20 9 1 - 30 19 12 1  | 91 151.433         | $1.47 \times 10^{-7}$    | 410.3           |
|                                       | 29 20 10 1 - 30 19 11 1 | 91 151.433         | $1.47 \times 10^{-7}$    | 410.3           |
|                                       | 27 19 8 0 - 28 18 11 0  | 91 182.665         | $1.14 \times 10^{-7}$    | 362.9           |
|                                       | 27 19 9 0 - 28 18 10 0  | 91 182.665         | $1.13 \times 10^{-7}$    | 362.9           |
|                                       | 14 3 11 1 - 13 4 10 1   | 91 186.341         | $6.58 \times 10^{-7}$    | 57.4            |
|                                       | 16 3 14 1 - 15 4 12 0   | 91 213.836         | $1.30 \times 10^{-7}$    | 71.5            |
|                                       | 14 3 11 0 - 13 4 10 0   | 91 224.675         | $4.15 \times 10^{-7}$    | 57.1            |
|                                       | 28 9 20 0 - 27 10 18 1  | 91 234.81          | $1.11 \times 10^{-7}$    | 239.8           |
|                                       | 10 5 5 0 - 10 4 6 0     | 91 244.026         | $1.81 \times 10^{-6}$    | 39.3            |
|                                       | 10 5 5 1 - 10 4 6 1     | 91 253.037         | $1.92 \times 10^{-6}$    | 39.7            |
|                                       | 28 9 19 0 - 27 10 17 1  | 91 267.756         | $1.10 \times 10^{-7}$    | 239.8           |
|                                       | 27 19 8 1 - 28 18 11 1  | 91 302.508         | $1.39 \times 10^{-7}$    | 363.2           |



Table B.2: continued.

| Species                               | Transition<br>J K L M   | Frequency<br>(MHz) | $A_{ij}$<br>( $s^{-1}$ ) | $E_{up}$<br>(K) |
|---------------------------------------|-------------------------|--------------------|--------------------------|-----------------|
|                                       | 27 19 9 1 - 28 18 10 1  | 91 302.508         | $1.39 \times 10^{-7}$    | 363.2           |
|                                       | 11 5 7 0 - 11 4 8 0     | 91 308.601         | $1.87 \times 10^{-6}$    | 44.7            |
|                                       | 11 5 7 1 - 11 4 8 1     | 91 321.795         | $2.05 \times 10^{-6}$    | 45.1            |
|                                       | 16 5 12 1 - 16 4 13 1   | 91 327.482         | $1.50 \times 10^{-6}$    | 79.7            |
|                                       | 25 18 7 0 - 26 17 10 0  | 91 335.784         | $1.06 \times 10^{-7}$    | 318.7           |
|                                       | 25 18 8 0 - 26 17 9 0   | 91 335.784         | $1.06 \times 10^{-7}$    | 318.7           |
|                                       | 18 4 15 1 - 17 5 12 1   | 91 340.39          | $4.62 \times 10^{-7}$    | 92.6            |
|                                       | 37 14 24 1 - 36 15 22 0 | 91 349.668         | $8.79 \times 10^{-8}$    | 442.3           |
|                                       | 37 14 23 1 - 36 15 21 0 | 91 349.672         | $8.79 \times 10^{-8}$    | 442.3           |
|                                       | 15 1 14 1 - 15 1 15 0   | 93 180.613         | $3.17 \times 10^{-7}$    | 59.9            |
|                                       | 18 2 16 1 - 17 4 14 1   | 93 181.585         | $4.49 \times 10^{-8}$    | 88.2            |
|                                       | 19 1 18 1 - 18 2 16 0   | 103 296.497        | $1.03 \times 10^{-7}$    | 92.8            |
|                                       | 25 7 19 0 - 24 8 17 1   | 103 307.653        | $2.11 \times 10^{-7}$    | 184.5           |
|                                       | 19 2 17 1 - 19 2 18 0   | 103 341.273        | $2.55 \times 10^{-7}$    | 97.4            |
|                                       | 17 6 11 0 - 17 5 13 1   | 103 365.434        | $4.16 \times 10^{-7}$    | 93.1            |
|                                       | 15 6 10 0 - 15 5 10 1   | 103 477.405        | $5.87 \times 10^{-7}$    | 76.8            |
|                                       | 30 10 21 1 - 29 11 19 0 | 103 489.245        | $1.47 \times 10^{-7}$    | 278.4           |
|                                       | 30 10 20 1 - 29 11 18 0 | 103 496.358        | $1.48 \times 10^{-7}$    | 278.4           |
| gGg-(CH <sub>2</sub> OH) <sub>2</sub> | 19 2 18 0 - 18 3 16 1   | 90 619.203         | $6.90 \times 10^{-7}$    | 91.9            |
|                                       | 9 5 4 1 - 9 4 5 1       | 90 625.64          | $3.63 \times 10^{-6}$    | 34.2            |
|                                       | 9 5 4 0 - 9 4 5 0       | 90 637.706         | $3.50 \times 10^{-6}$    | 34.1            |
|                                       | 22 6 17 0 - 22 5 17 1   | 90 710.878         | $3.12 \times 10^{-6}$    | 141.6           |
|                                       | 9 5 5 1 - 9 4 6 1       | 90 750.006         | $3.54 \times 10^{-6}$    | 34.2            |
|                                       | 9 5 5 0 - 9 4 6 0       | 90 761.349         | $3.62 \times 10^{-6}$    | 34.1            |
|                                       | 17 3 15 0 - 16 4 13 1   | 90 849.293         | $1.24 \times 10^{-6}$    | 78.8            |
|                                       | 19 15 4 1 - 20 14 6 0   | 90 855.162         | $1.57 \times 10^{-7}$    | 202.0           |
|                                       | 19 15 5 1 - 20 14 7 0   | 90 855.162         | $1.57 \times 10^{-7}$    | 202.0           |
|                                       | 8 5 3 1 - 8 4 4 1       | 90 862.788         | $3.34 \times 10^{-6}$    | 29.8            |
|                                       | 8 5 3 0 - 8 4 4 0       | 90 874.028         | $3.28 \times 10^{-6}$    | 29.7            |
|                                       | 8 5 4 1 - 8 4 5 1       | 90 911.505         | $3.31 \times 10^{-6}$    | 29.8            |
|                                       | 8 5 4 0 - 8 4 5 0       | 90 922.458         | $3.32 \times 10^{-6}$    | 29.7            |
|                                       | 16 1 15 0 - 16 0 16 0   | 90 930.932         | $1.45 \times 10^{-6}$    | 66.7            |
|                                       | 11 5 7 1 - 11 4 7 0     | 90 988.303         | $3.83 \times 10^{-6}$    | 44.5            |
|                                       | 7 5 2 1 - 7 4 3 1       | 91 016.495         | $2.96 \times 10^{-6}$    | 25.9            |
|                                       | 7 5 2 0 - 7 4 3 0       | 91 027.312         | $2.92 \times 10^{-6}$    | 25.8            |
|                                       | 7 5 3 1 - 7 4 4 1       | 91 032.962         | $2.95 \times 10^{-6}$    | 25.9            |
|                                       | 7 5 3 0 - 7 4 4 0       | 91 043.681         | $2.93 \times 10^{-6}$    | 25.8            |
|                                       | 4 3 2 1 - 3 2 1 1       | 91 101.828         | $4.93 \times 10^{-6}$    | 9.3             |
|                                       | 6 5 1 1 - 6 4 2 1       | 91 113.072         | $2.40 \times 10^{-6}$    | 22.5            |
|                                       | 4 3 2 0 - 3 2 1 0       | 91 113.703         | $4.72 \times 10^{-6}$    | 9.3             |
|                                       | 17 14 3 1 - 18 13 5 0   | 91 113.915         | $1.32 \times 10^{-7}$    | 169.9           |
|                                       | 17 14 4 1 - 18 13 6 0   | 91 113.915         | $1.31 \times 10^{-7}$    | 169.9           |
|                                       | 6 5 2 1 - 6 4 3 1       | 91 117.61          | $2.39 \times 10^{-6}$    | 22.5            |
|                                       | 6 5 1 0 - 6 4 2 0       | 91 123.664         | $2.37 \times 10^{-6}$    | 22.4            |
|                                       | 17 5 12 0 - 17 4 14 1   | 91 125.215         | $4.19 \times 10^{-6}$    | 87.2            |
|                                       | 6 5 2 0 - 6 4 3 0       | 91 128.176         | $2.37 \times 10^{-6}$    | 22.4            |
|                                       | 16 1 15 1 - 16 0 16 1   | 91 152.424         | $1.69 \times 10^{-6}$    | 66.8            |
|                                       | 5 5 0 1 - 5 4 1 1       | 91 170.801         | $1.52 \times 10^{-6}$    | 19.5            |
|                                       | 5 5 1 1 - 5 4 2 1       | 91 171.716         | $1.52 \times 10^{-6}$    | 19.5            |
|                                       | 41 6 35 1 - 40 9 32 1   | 91 177.349         | $1.31 \times 10^{-7}$    | 446.6           |
|                                       | 5 5 0 0 - 5 4 1 0       | 91 181.28          | $1.50 \times 10^{-6}$    | 19.5            |
|                                       | 5 5 1 0 - 5 4 2 0       | 91 182.189         | $1.50 \times 10^{-6}$    | 19.5            |
|                                       | 30 5 25 0 - 30 5 26 1   | 91 231.701         | $3.36 \times 10^{-7}$    | 244.5           |
|                                       | 41 6 35 0 - 40 9 32 0   | 91 257.694         | $1.21 \times 10^{-7}$    | 446.6           |
|                                       | 18 5 14 1 - 18 4 15 1   | 91 262.747         | $4.24 \times 10^{-6}$    | 96.0            |
|                                       | 18 5 14 0 - 18 4 15 0   | 91 268.437         | $4.70 \times 10^{-6}$    | 96.0            |

Table B.2: continued.

| Species                            | Transition<br>J K L M | Frequency<br>(MHz) | $A_{ij}$<br>( $s^{-1}$ ) | $E_{up}$<br>(K) |
|------------------------------------|-----------------------|--------------------|--------------------------|-----------------|
|                                    | 13 5 8 1 - 13 4 10 0  | 91 275.54          | $3.05 \times 10^{-6}$    | 56.7            |
|                                    | 14 5 9 1 - 14 4 11 0  | 91 280.948         | $3.02 \times 10^{-6}$    | 63.6            |
|                                    | 18 3 16 0 - 18 1 17 1 | 91 306.616         | $1.57 \times 10^{-6}$    | 87.5            |
|                                    | 9 2 8 1 - 8 2 7 0     | 91 332.324         | $6.59 \times 10^{-6}$    | 23.8            |
|                                    | 31 7 24 1 - 31 6 25 1 | 91 355.815         | $6.00 \times 10^{-6}$    | 268.3           |
|                                    | 15 13 2 1 - 16 12 4 0 | 91 361.122         | $1.01 \times 10^{-7}$    | 140.7           |
|                                    | 15 13 3 1 - 16 12 5 0 | 91 361.122         | $1.01 \times 10^{-7}$    | 140.7           |
|                                    | 9 4 5 1 - 8 4 4 0     | 93 162.746         | $5.77 \times 10^{-6}$    | 29.8            |
|                                    | 17 3 15 1 - 16 4 13 0 | 93 172.871         | $1.32 \times 10^{-6}$    | 78.9            |
|                                    | 18 5 13 0 - 18 4 15 1 | 93 190.697         | $3.45 \times 10^{-6}$    | 96.1            |
|                                    | 10 4 7 1 - 9 4 6 0    | 103 372.306        | $8.30 \times 10^{-6}$    | 34.7            |
|                                    | 18 4 14 0 - 18 3 16 1 | 103 426.616        | $1.89 \times 10^{-6}$    | 92.5            |
|                                    | 22 4 19 0 - 22 2 20 1 | 103 438.467        | $5.12 \times 10^{-6}$    | 131.6           |
|                                    | 22 2 21 0 - 21 2 19 0 | 103 457.183        | $1.01 \times 10^{-7}$    | 121.0           |
|                                    | 19 3 17 0 - 18 4 15 1 | 103 488.002        | $1.74 \times 10^{-6}$    | 96.6            |
| D <sub>2</sub> CO                  | 5 1 4 - 5 1 5         | 91 246.233         | $1.61 \times 10^{-6}$    | 49.6            |
| t-HCOOH                            | 34 4 30 - 34 4 31     | 103 423.53         | $2.60 \times 10^{-7}$    | 700.5           |
| c-C <sub>2</sub> H <sub>4</sub> O  | 11 6 5 - 11 5 6       | 90 842.056         | $8.21 \times 10^{-6}$    | 137.2           |
|                                    | 21 14 7 - 21 13 8     | 91 160.793         | $1.21 \times 10^{-5}$    | 492.8           |
| c-C <sub>2</sub> H <sub>3</sub> DO | 9 5 5 - 9 3 6         | 90 667.609         | $1.17 \times 10^{-7}$    | 83.6            |
|                                    | 7 2 5 - 7 2 6         | 90 683.057         | $9.45 \times 10^{-8}$    | 48.3            |
|                                    | 7 2 5 - 7 1 6         | 90 710.475         | $4.70 \times 10^{-6}$    | 48.3            |
|                                    | 10 8 2 - 10 7 3       | 90 781.87          | $6.42 \times 10^{-6}$    | 113.1           |
|                                    | 13 8 6 - 12 11 1      | 90 852.748         | $1.17 \times 10^{-9}$    | 174.4           |
|                                    | 12 7 6 - 11 10 1      | 91 140.581         | $1.69 \times 10^{-9}$    | 147.5           |
|                                    | 13 2 11 - 12 5 8      | 91 153.128         | $1.10 \times 10^{-8}$    | 141.1           |
|                                    | 13 3 11 - 12 4 8      | 91 366.508         | $1.10 \times 10^{-8}$    | 141.1           |
| HC <sub>3</sub> N                  | 10 - 9                | 90 979.023         | $5.81 \times 10^{-5}$    | 24.0            |
| CH <sub>3</sub> CH <sub>2</sub> CN | 35 5 31 - 36 2 34     | 90 800.771         | $6.07 \times 10^{-8}$    | 299.2           |
|                                    | 49 7 43 - 50 5 46     | 90 949.453         | $2.17 \times 10^{-8}$    | 581.9           |
|                                    | 58 8 51 - 59 6 54     | 90 998.392         | $2.24 \times 10^{-8}$    | 807.6           |
|                                    | 27 2 25 - 27 2 26     | 91 008.34          | $5.49 \times 10^{-7}$    | 169.8           |
|                                    | 29 3 26 - 29 2 27     | 91 018.22          | $5.25 \times 10^{-6}$    | 199.1           |
|                                    | 48 7 41 - 47 8 40     | 91 161.765         | $1.09 \times 10^{-6}$    | 560.8           |
|                                    | 61 3 58 - 60 5 55     | 91 196.7           | $3.17 \times 10^{-8}$    | 828.0           |
|                                    | 36 2 34 - 35 4 31     | 91 281.468         | $7.96 \times 10^{-8}$    | 294.8           |
|                                    | 35 3 33 - 36 1 36     | 91 284.048         | $5.56 \times 10^{-9}$    | 280.5           |
|                                    | 14 3 12 - 15 0 15     | 91 342.464         | $3.11 \times 10^{-8}$    | 55.2            |
|                                    | 35 3 33 - 36 0 36     | 91 350.299         | $2.83 \times 10^{-8}$    | 280.5           |
|                                    | 39 2 37 - 40 1 40     | 93 156.345         | $2.49 \times 10^{-8}$    | 343.8           |
|                                    | 39 2 37 - 40 0 40     | 93 181.535         | $4.84 \times 10^{-9}$    | 343.8           |
|                                    | 21 7 15 - 22 6 16     | 103 384.573        | $1.23 \times 10^{-6}$    | 153.8           |
|                                    | 21 7 14 - 22 6 17     | 103 385.42         | $1.23 \times 10^{-6}$    | 153.8           |
|                                    | 60 4 57 - 59 5 54     | 103 417.147        | $2.63 \times 10^{-7}$    | 802.3           |
| HOCH <sub>2</sub> CN               | 38 2 36 0 - 39 1 39 0 | 90 597.603         | $5.26 \times 10^{-8}$    | 338.5           |
|                                    | 25 2 23 0 - 25 1 24 0 | 90 619.344         | $4.38 \times 10^{-6}$    | 151.6           |
|                                    | 18 4 14 0 - 18 3 16 1 | 90 635.379         | $2.87 \times 10^{-6}$    | 98.0            |
|                                    | 36 8 29 0 - 37 7 30 0 | 90 753.122         | $1.17 \times 10^{-6}$    | 383.8           |
|                                    | 36 8 28 0 - 37 7 31 0 | 90 757.105         | $1.17 \times 10^{-6}$    | 383.8           |
|                                    | 19 4 15 0 - 19 3 17 1 | 90 808.881         | $2.86 \times 10^{-6}$    | 106.4           |
|                                    | 49 5 45 1 - 50 2 48 1 | 90 829.279         | $8.35 \times 10^{-8}$    | 583.4           |
|                                    | 23 4 19 1 - 24 2 22 1 | 90 918.82          | $1.95 \times 10^{-7}$    | 149.9           |
|                                    | 29 5 25 1 - 30 4 27 0 | 90 932.471         | $1.27 \times 10^{-6}$    | 232.8           |
|                                    | 23 2 21 0 - 23 1 23 1 | 90 938.751         | $8.97 \times 10^{-7}$    | 129.5           |
|                                    | 8 0 8 1 - 8 1 8 0     | 90 948.488         | $6.84 \times 10^{-6}$    | 21.3            |
|                                    | 8 1 8 1 - 7 2 6 0     | 90 973.549         | $8.01 \times 10^{-7}$    | 22.3            |

Table B.2: continued.

| Species             | Transition<br>J K L M     | Frequency<br>(MHz) | $A_{ij}$<br>( $s^{-1}$ ) | $E_{up}$<br>(K) |
|---------------------|---------------------------|--------------------|--------------------------|-----------------|
|                     | 20 4 16 0 - 20 3 18 1     | 91 039.63          | $2.87 \times 10^{-6}$    | 115.3           |
|                     | 42 2 40 0 - 41 4 37 0     | 91 089.387         | $1.69 \times 10^{-7}$    | 410.4           |
|                     | 56 7 50 1 - 55 8 47 1     | 91 170.271         | $1.30 \times 10^{-6}$    | 780.4           |
|                     | 49 5 45 0 - 50 2 48 0     | 91 212.431         | $1.20 \times 10^{-7}$    | 578.4           |
|                     | 10 0 10 1 - 9 0 9 1       | 91 244.602         | $2.25 \times 10^{-5}$    | 29.6            |
|                     | 35 6 30 1 - 36 5 32 0     | 91 280.978         | $1.27 \times 10^{-6}$    | 334.4           |
|                     | 10 0 10 0 - 9 0 9 0       | 91 282.104         | $2.27 \times 10^{-5}$    | 24.2            |
|                     | 29 2 27 1 - 29 2 28 1     | 91 307.51          | $1.12 \times 10^{-7}$    | 206.3           |
|                     | 21 4 17 0 - 21 3 19 1     | 91 343.484         | $2.87 \times 10^{-6}$    | 124.6           |
|                     | 34 3 32 0 - 33 4 29 0     | 93 175.688         | $1.03 \times 10^{-6}$    | 276.0           |
|                     | 16 1 15 0 - 15 1 15 1     | 93 179.831         | $4.57 \times 10^{-7}$    | 62.8            |
|                     | 30 9 21 0 - 31 8 23 1     | 93 190.634         | $9.50 \times 10^{-7}$    | 318.3           |
|                     | 30 9 22 0 - 31 8 24 1     | 93 190.64          | $9.50 \times 10^{-7}$    | 318.3           |
|                     | 35 2 33 0 - 34 3 31 1     | 103 318.063        | $3.15 \times 10^{-6}$    | 288.9           |
|                     | 45 3 42 1 - 45 3 42 0     | 103 318.312        | $9.15 \times 10^{-8}$    | 482.2           |
|                     | 59 9 51 1 - 58 10 49 0    | 103 334.357        | $1.76 \times 10^{-6}$    | 901.2           |
|                     | 59 9 50 1 - 58 10 48 0    | 103 341.424        | $1.76 \times 10^{-6}$    | 901.2           |
|                     | 20 2 18 0 - 19 2 18 1     | 103 352.311        | $7.48 \times 10^{-8}$    | 99.7            |
|                     | 21 4 17 1 - 22 3 19 0     | 103 384.207        | $1.71 \times 10^{-6}$    | 130.0           |
|                     | 32 2 30 1 - 32 2 30 0     | 103 402.141        | $1.77 \times 10^{-6}$    | 248.2           |
|                     | 27 4 23 1 - 26 5 21 0     | 103 421.493        | $1.71 \times 10^{-6}$    | 195.2           |
|                     | 57 7 50 0 - 56 8 49 0     | 103 437.673        | $1.87 \times 10^{-6}$    | 800.8           |
|                     | 46 8 38 1 - 47 7 40 0     | 103 440.794        | $1.79 \times 10^{-6}$    | 572.8           |
|                     | 48 4 44 1 - 48 4 44 0     | 103 506.105        | $1.08 \times 10^{-7}$    | 552.9           |
| NH <sub>2</sub> CHO | 15 3 12 - 16 1 15         | 91 136.103         | $4.85 \times 10^{-8}$    | 149.5           |
|                     | 36 5 32 - 35 6 29         | 103 296.485        | $7.38 \times 10^{-7}$    | 755.7           |
|                     | 20 5 16 - 21 4 17         | 103 446.144        | $7.16 \times 10^{-7}$    | 288.6           |
| CH <sub>3</sub> SH  | 1 -1 1 1 - 0 0 0 1        | 90 637.359         | $7.97 \times 10^{-7}$    | 5.8             |
|                     | 12 -1 12 4 - 11 -2 10 4   | 91 128.19          | $3.80 \times 10^{-7}$    | 571.2           |
|                     | 9 1 8 1 - 9 0 9 1         | 103 389.812        | $2.55 \times 10^{-6}$    | 61.0            |
|                     | 12 3 9 1 - 13 2 11 1      | 103 399.789        | $5.79 \times 10^{-7}$    | 133.6           |
|                     | 8 0 8 0 - 7 1 6 0         | 103 504.193        | $1.54 \times 10^{-6}$    | 43.7            |
|                     | 27 5 22 -3 - 26 6 20 -3   | 103 508.935        | $5.40 \times 10^{-7}$    | 870.7           |
|                     | 27 -5 23 -3 - 26 -6 21 -3 | 103 509.321        | $5.40 \times 10^{-7}$    | 870.7           |