# 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  $(\sim 0.8 \text{ mm})$ , it is generally more difficult to detect larger molecules than at longer wavelengths  $(\sim 3 \text{ mm})$  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  $\gtrsim 6\sigma$  level,  $\sim$ 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  $\sim$ 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 - HOCH2CH(OH)CH2OH, 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 -21 NH<sub>2</sub>CH<sub>2</sub>COOH, Ioppolo et al. 2021). However, there is a lot 22 of debate regarding the ice or gas-phase formation of particu-23 lar COMs (e.g., Ceccarelli et al. 2022). Two examples of these 24 species are formamide (NH<sub>2</sub>CHO) and acetaldehyde (CH<sub>3</sub>CHO) 25 for which both gas and ice formation pathways are suggested 26 (e.g., Jones et al. 2011; Barone et al. 2015; Vazart et al. 2020; 27 Chuang et al. 2020, 2021, 2022; Fedoseev et al. 2022; Garrod 28 et al. 2022). To obtain clues as to the formation mechanism of 29 COMs from an observational perspective, it is possible to search 30 for the solid state signatures of COMs in ices (Schutte et al. 31 1999; Öberg et al. 2011) with telescopes such as the James Webb 32 Space Telescope (Yang et al. 2022; McClure et al. 2023; Rocha 33 et al. in prep.) using laboratory spectra available from, for ex-34 ample, the Leiden Ice Database for Astrochemistry (Rocha et al. 35 2022) and to examine the gas-phase correlations between dif-36 ferent COMs in large samples of sources (Belloche et al. 2020; 37 Coletta et al. 2020; Jørgensen et al. 2020; Nazari et al. 2022a; 38 Taniguchi et al. 2023; Chen et al. 2023). However, observations 39 and models show that physical effects such as the source struc-40 ture or dust optical depth could affect the snowline locations, 41

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gas-phase emission, and column density correlations of simple 42 and complex molecules (Jørgensen et al. 2002; Persson et al. 43 2016; De Simone et al. 2020; Nazari et al. 2022b; Murillo et al. 44 2022a; Nazari et al. 2023a,b). Hence, interpretations of COM 45 formation routes based on gas-phase observations can be af-46 fected by these physical factors. For example, an anticorrelation 47 between column densities of two species (or a large scatter in the 48 column density ratios) could have a physical origin rather than a 49 chemical origin. 50

Among the low-mass protostars, the IRAS16293-2422 51 (IRAS16293 hereafter) triple protostellar system (Wootten 1989; 52 Maureira et al. 2020) is one of the closest protostars, and one 53 of the richest and most well-studied objects from a chemical 54 perspective. The first detection of methanol (CH<sub>3</sub>OH; the sim-55 plest COM) toward a low-mass protostar was carried out by van 56 Dishoeck et al. (1995) for this system. Since then, its chem-57 58 istry and in particular the COMs in this system have been stud-59 ied in more detail (Cazaux et al. 2003; Butner et al. 2007; Bisschop et al. 2008; Ceccarelli et al. 2010; Jørgensen et al. 60 2011; Jørgensen et al. 2012; Kahane et al. 2013; Jaber et al. 61 2014). More recently, the Protostellar Interferometric Line Sur-62 vey (PILS; Jørgensen et al. 2016) studied IRAS16293 in Band 63 64 7 (~329.147 – 362.896 GHz) of the Atacama Large Millimeter/submillimeter Array (ALMA). This survey detected many 65 COMs for the first time in the ISM, adding further information 66 on complexity in space (Coutens et al. 2016; Lykke et al. 2017; 67 68 Calcutt et al. 2018a; Jørgensen et al. 2018; Manigand et al. 2019; Manigand et al. 2021; Coutens et al. 2022). 69

However, a limitation of higher-frequency observations of 70 ALMA ( $\sim$ 330 GHz) is the higher degree of line blending. The 71 reason is that for observations probing the same gas, the line 72 73 width - although constant in velocity space - increases in fre-74 quency space (Jørgensen et al. 2020). Therefore, the detection of 75 larger COMs with more than eight atoms, which have relatively 76 weak lines, is expected to be easier at lower frequencies. Moreover, the heavier molecules have their Boltzmann distribution 77 peak at lower frequencies than the lighter molecules at the same 78 excitation temperature, and thus their lines are stronger at lower 79 frequencies and they are more easily detected at long wavelength 80 observations. On the other hand, the Boltzmann peak moves to 81 the higher frequencies for higher temperatures (see Fig. 2 of 82 Herbst & van Dishoeck 2009). Therefore, if the large molecules 83 are thermally sublimated in the inner hot regions around the pro-84 tostar (tracing warm or hot regions), it is difficult to observe these 85 larger species even at low frequencies (although favored), unless 86 the data are sensitive enough, which can be achieved at the ex-87 pense of the angular resolution and longer integration times. The 88 combination of the increase in line width in frequency space and 89 the Boltzmann distribution peak of the lighter molecules being 90 at higher frequencies also lead to spectra being more crowded, 91 and thus it is more difficult to detect large molecules at high fre-92 quencies. 93

Moreover, dust optical depth effects could be an impor-94 tant issue at higher-frequency ALMA Bands 6 (~240 GHz) and 95 7 (~330 GHz). This is because of the larger dust opacity of 96  $\sim$ 1 mm-sized grains at shorter wavelengths (i.e, higher frequen-97 cies). For example, López-Sepulcre et al. (2017) found that NGC 98 1333 IRAS 4A1 in Perseus does not host any COMs when 99 searched for with ALMA and the Plateau de Bure Interferom-100 eter. However, later, De Simone et al. (2020) detected methanol 101 around this source at longer wavelengths with the Very Large 102 Array (VLA). Another example is the ring-shaped structure of 103 methanol around the dust continuum in the massive protostellar 104 system 693050 (also known as G301.1364-00.2249) observed 105

by van Gelder et al. (2022b) at ~220 GHz with ALMA, which 106 indicates dust attenuation on-source. 107

For this work, we used the deep Band 3 ALMA observa-108 tions of IRAS16293 B to search for larger species (more than 109 eight atoms). This dataset was specifically optimized to hunt for 110 molecules such as glycerol and i- and n-propanol. Although the 111 main aim is to specifically hunt for large molecules, we identi-112 fied as many molecules as possible from the Cologne Database 113 for Molecular Spectroscopy (CDMS; Müller et al. 2001; Müller 114 et al. 2005) and the Jet Propulsion Laboratory database (JPL; 115 Pickett et al. 1998) in our data. We fit the spectrum to derive 116 the column densities and excitation temperatures of the detected 117 species and we compared our results with those of PILS in 118 Band 7. In particular, we examined whether dust attenuation is 119 important for column densities and their ratios with respect to 120 methanol (typically used as a reference species). 121

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.

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# 2. Observations and methods

2.1. Data

This paper uses the data of IRAS16293 B taken with ALMA in 130 Band 3 (project code: 2017.1.00518.S; PI: E. F. van Dishoeck). 131 For more information on the data calibration, reduction, and 132 imaging, as well as the first results on the gas accretion flow 133 in the IRAS16293 system, readers can refer to Murillo et al. 134 (2022b); here we give a brief description of the data. We used 135 the data with the configuration C43-4, which were calibrated 136 with the CASA pipeline (McMullin et al. 2007) and then self-137 calibrated with CASA. Continuum subtraction was done on the 138 self-calibrated image datacubes using STATCONT (Sánchez-139 Monge et al. 2018). 140

The data have an angular resolution of  $\sim 0.9'' \times 0.7''$ , which is 141 larger than that of PILS ( $\sim 0.5''$ ). The frequency ranges covered 142 were ~90.59 - 91.41 GHz (continuum), ~93.14 - 93.20 GHz, 143 and ~103.28 - 103.52 GHz. After conversion of the flux to 144 brightness temperature, the rms found from line-free regions in 145 each spectral window was ~0.1 K, ~0.3 K, and 0.2 K (compara-146 ble to PILS), respectively, following a 171.7 minute on-source 147 integration time. The spectral resolution was  $0.805 \,\mathrm{km \, s^{-1}}$ , 148  $0.049 \text{ km s}^{-1}$ , and  $0.088 \text{ km s}^{-1}$ . Given that the lines have a full 149 width at half maximum (FWHM) of  $\sim 1 - 2 \text{ km s}^{-1}$ , some lines 150 are not fully resolved in the continuum window. The frequency 151 range was optimized to cover transitions of larger species such 152 as glycerol as well as i- and n-propanol. It also serendipitously 153 covered transitions from other oxygen- and nitrogen-bearing 154 COMs including glycolaldehyde (CH<sub>2</sub>OHCHO), propanal (g-155  $C_2H_5CHO$ ), and glycolonitrile (HOCH<sub>2</sub>CN). The spectrum of 156 IRAS16293 B (Fig. 1) was extracted from the same 0.5" offset 157 position from the continuum peak of B that was used in many 158 of the works from ALMA-PILS ( $\alpha_{J2000} = 16^{h}32^{m}22^{s}.58$  and 159  $\delta_{J2000} = -24^{\circ}28'32.8''$ , Coutens et al. 2016; Jørgensen et al. 160 2018; Calcutt et al. 2018b). Maps of a few common species trac-161 ing cold gas structures are presented in Murillo et al. (2022b). 162



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

For this work, we identified as many molecules as possible us-164 ing the CASSIS<sup>1</sup> spectral analysis tool (Vastel et al. 2015). We 165 consider a molecule as detected if it has at least three lines at 166 a peak of the  $\geq 3\sigma$  level. We also report column densities of 167 the molecules that have one or two detected lines without any 168 overprediction of the emission in the spectrum. These column 169 densities are only tentative and not as robust as those found for 170 171 molecules with many detected lines because of the limited frequency coverage, but they should be reliable for the most abun-172 dant and common molecules such as <sup>13</sup>CH<sub>3</sub>OH. Using CAS-173 SIS, we fit for the identified molecules. In the fitting procedure, 174 the spectrum was considered as a whole; and all the lines of 175 a molecule were fitted simultaneously assuming local thermo-176 dynamic equilibrium (LTE) conditions. The fitting followed a 177 similar procedure as the fit-by-eye method used in Nazari et al. 178 (2022a). This includes varying the column densities (N) and 179 excitation temperatures  $(T_{ex})$  in the LTE models to produce a 180 synthetic spectrum that matches the data (for more informa-181 tion on this process, see below). The line lists were taken from 182 the CDMS (Müller et al. 2001; Müller et al. 2005) or the JPL 183 184 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 unblended line(s) of each molecule. Then it was fixed to that 188 value when the column density and excitation temperature were 189 being determined. The FWHM for all considered species is 190  $\sim 1.8 \pm 0.5 \,\mathrm{km \, s^{-1}}$ , except for (formic acid) t-HCOOH, which 191 is slightly lower (i.e.,  $\sim 1 \text{ km s}^{-1}$ ). The typical FWHM here is 192  $\sim 1.5 - 2$  times larger than the typical FWHM found in PILS 193  $(\sim 1 \text{ km s}^{-1})$ . However, the spectral resolution for the continuum 194 spectral window (i.e., the major spectral window where most 195 lines lie; Fig. B.1) is  $\sim 0.8 \text{ km s}^{-1}$  in this work. This implies 196 that not all lines are spectrally resolved. Therefore, the higher 197 198 FWHM measured here could be due to this low spectral reso-199 lution. The excitation temperature was only fitted if there were enough ( $\geq 2$ ) detected lines of a molecule with a range of  $E_{up}$ 200 (e.g.,  $\sim 100 - 400$  K). The typical uncertainty on the excitation 201 temperature is  $\sim \pm 50$  K. If not enough lines with a range of 202  $E_{\rm up}$  were detected, the temperature is fixed to 100 K, which is 203 similar to excitation temperatures assumed or found for many 204

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  $T_{ex}$ . 212 Deuterated methanol, CH<sub>2</sub>DOH, has three detected lines, with 213 upper energy levels of ~10 K, ~100 K, and ~400 K. It was not 214 possible to fit all three lines of this molecule with a single excita-215 tion 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 ~100 K line bet-218 ter than the other two. For  $aGg'-(CH_2OH)_2$ , we note that again a 219 single temperature cannot fit all of its lines. In particular, the line 220 at 90.593 GHz with  $E_{up} = 19$  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

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

<sup>&</sup>lt;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.

# 253 3. Results

## 254 3.1. Deep search and the considered species

The spectrum of IRAS16293 B at ~3 mm wavelengths is line 255 rich and crowded (see Fig. 1 for an overview). In total, 16 256 molecules were detected and 15 were tentatively detected (see 257 Table 1). Ratios of the detected molecules with respect to 258 methanol are presented in the left panel of Fig. 2 (see Sect. 4.2.3 259 for a discussion on the comparison with PILS). Among these 260 species, many "standard" COMs such as methanol (CH<sub>3</sub>OH), 261 ethanol (CH<sub>3</sub>CH<sub>2</sub>OH), ethyl cyanide (CH<sub>3</sub>CH<sub>2</sub>CN), acetalde-262 hyde (CH<sub>3</sub>CHO), methyl formate (CH<sub>3</sub>OCHO), and dimethyl 263 ether (CH<sub>3</sub>OCH<sub>3</sub>) with some of their isotopologues are appar-264 ent. The frequency range did not cover transitions of CH<sub>3</sub>CN and 265 HNCO or their isotopologues. We also detected one carbon chain 266 molecule, cyanoacetylene (HCCCN). It should be noted that the 267 frequency range of the observations covers HC<sub>5</sub>N transitions, but 268 this carbon chain was not detected toward IRAS16293 B. It was, 269 however, detected  ${\sim}12^{\prime\prime}$  off-source to the west of IRAS16293 B 270 (Murillo et al. 2022b). 271

This dataset was specifically taken to search for large species 272 due to the expected lower line density and line confusion in 273 Band 3 in comparison with Band 7 used for PILS. More-274 over, at the same excitation temperature, heavier molecules have 275 their Boltzmann distribution peak at lower frequencies, which 276 increases the chance of detecting them in Band 3. Particu-277 278 larly, the frequency windows were selected to search for glycerol (HOCH<sub>2</sub>CH(OH)CH<sub>2</sub>OH) and propanol (C<sub>3</sub>H<sub>7</sub>OH). Iso-279 propanol (i-C<sub>3</sub>H<sub>7</sub>OH) and normal-propanol (n-C<sub>3</sub>H<sub>7</sub>OH) have 280 been detected previously in the ISM (Belloche et al. 2022; 281 Jiménez-Serra et al. 2022), although not yet in IRAS16293 282 B (Taquet et al. 2018). In addition to these molecules, we 283 searched for and detected large and complex species such 284 as aGg'- and gGg'-ethylene glycol (CH<sub>2</sub>OH)<sub>2</sub>, glycolaldehyde 285 (CH<sub>2</sub>OHCHO), and acetone (CH<sub>3</sub>COCH<sub>3</sub>). 286

Table B.1 presents the upper limits of the molecules we 287 searched for but do not detect, including glycerol and iso-288 propanol. The largest molecule that we searched for is cyanon-289 aphthalene ( $C_{10}H_7CN$ ; McNaughton et al. 2018) and its upper 290 limit is given in Table B.1. Figures 3, B.2, and B.3 present the 291 lines of g-Isopropanol, Ga-n-propanol, and G'Gg'gg'-Glycerol 292 with the model upper limits. We note that in Fig. 3, the lines that 293 seem to agree well with the data in the first two panels are well 294 explained with other molecules (see the cyan line as the total fit-295 ted model for the detected or tentatively detected species), and 296 thus they could not be the lines of g-Isopropanol. Moreover, the 297 line at around 91.345 GHz overestimates the data. The ratio of 298 measured upper limits with respect to methanol are presented in 299 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 300 301 seen for the detected molecules (left panel of Fig. 2). 302

The line density of the lines detected at  $\geq 6\sigma$  level in Band 3 (~100 GHz) data is one per ~8.5 MHz (see Fig. B.1 for the variations in line density across the frequency range), while the line density is one per ~3.5 MHz in Band 7 (~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 ~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	Ν	T <sub>ex</sub>	$N_{\rm X}/N_{\rm CH_3OH}$	# Detected
	$(cm^{-2})$	(K)		lines
<sup>13</sup> CH <sub>3</sub> OH	$1.2^{+0.4}_{-0.2} \times 10^{17}$	$130^{+30}_{-20}$	$1.5^{+0.7}_{-0.4} \times 10^{-2}$	2
CH <sub>2</sub> DOH	$1.5^{+0.1}_{-0.3} \times 10^{17}$	[170]	$1.8^{+0.6}_{-0.5} \times 10^{-2}$	3
CHD <sub>2</sub> OH	$1.9^{+0.4}_{-0.3} \times 10^{17}$	$170^{+40}_{-40}$	$2.3^{+0.9}_{-0.6} \times 10^{-2}$	9
CD <sub>3</sub> OH	$5.6^{+0.7}_{-0.9} \times 10^{16}$	[170]	$6.9^{+2.4}_{-1.8} \times 10^{-3}$	1
CH <sub>3</sub> CHO	$3.5^{+0.2}_{-0.4} \times 10^{16}$	$70^{+20}_{-10}$	$4.3^{+1.5}_{-1.0} \times 10^{-3}$	3
<sup>13</sup> CH <sub>3</sub> CHO	$2.1^{+0.3}_{-0.3} \times 10^{15}$	[100]	$2.6^{+0.9}_{-0.7} \times 10^{-4}$	2
CH <sub>2</sub> DCHO	$4.0^{+0.5}_{-0.5} \times 10^{15}$	[100]	$4.9^{+1.7}_{-1.2} \times 10^{-4}$	2
CH <sub>3</sub> CDO	$5.0^{+2.0}_{-2.0} \times 10^{15}$	$110^{+30}_{-30}$	$6.1^{+3.2}_{-2.8} \times 10^{-4}$	3
CHD <sub>2</sub> CHO	$3.0^{+0.5}_{-0.8} \times 10^{15}$	[100]	$3.7^{+1.4}_{-1.2} \times 10^{-4}$	3
CH <sub>3</sub> COOH	$1.0^{+0.6}_{-0.2} \times 10^{16}$	$170^{+30}_{-70}$	$1.2^{+0.8}_{-0.4} \times 10^{-3}$	3
CH <sub>2</sub> OHCHO	$4.6^{+0.6}_{-0.6} \times 10^{16}$	$280^{+20}_{-40}$	$5.6^{+2.0}_{-1.4} \times 10^{-3}$	6
<sup>13</sup> CH <sub>2</sub> OHCHO	$\sim 2.0 \times 10^{15}$	[280]	$\sim 2.4 \times 10^{-4}$	2
CHDOHCHO	$2.5^{+0.8}_{-0.8} \times 10^{15}$	$120^{+50}_{-50}$	$3.1^{+1.5}_{-1.2} \times 10^{-4}$	4
CH <sub>3</sub> CH <sub>2</sub> OH	$6.2^{+0.8}_{-0.7}  imes 10^{16}$	$170^{+20}_{-20}$	$7.6^{+2.7}_{-1.8} \times 10^{-3}$	5
a-a-CH <sub>2</sub> DCH <sub>2</sub> OH	$2.4^{+0.5}_{-0.3} \times 10^{16}$	[170]	$3.0^{+1.1}_{-0.7} \times 10^{-3}$	1
a-CH <sub>3</sub> CHDOH	$2.1^{+0.4}_{-0.3} \times 10^{16}$	[170]	$2.5^{+1.0}_{-0.6}  imes 10^{-3}$	3
CH <sub>3</sub> OCH <sub>3</sub>	$8.5^{+2.5}_{-2.5}  imes 10^{16}$	$100^{+20}_{-20}$	$1.0^{+0.5}_{-0.4}  imes 10^{-2}$	10
CH <sub>3</sub> OCHO	$1.0^{+0.1}_{-0.2} \times 10^{17}$	$140^{+20}_{-30}$	$1.2^{+0.4}_{-0.4} \times 10^{-2}$	10
aGg'-(CH <sub>2</sub> OH) <sub>2</sub>	$\sim 1.4 \times 10^{17}$	[160]	$\sim 1.7 \times 10^{-2}$	15
gGg'-(CH <sub>2</sub> OH) <sub>2</sub>	$5.0^{+1.7}_{-1.4}  imes 10^{16}$	$160^{+40}_{-40}$	$6.1^{+2.9}_{-2.1}  imes 10^{-3}$	15
$D_2CO$	$6.9^{+0.6}_{-0.6}  imes 10^{15}$	[100]	$8.5^{+2.9}_{-1.9}  imes 10^{-4}$	1
HCCCN	$6.2^{+0.9}_{-0.8}  imes 10^{13}$	[100]	$7.6^{+2.8}_{-1.8}  imes 10^{-6}$	1
CH <sub>3</sub> CH <sub>2</sub> CN	$1.4^{+0.2}_{-0.1} \times 10^{16}$	[100]	$1.8^{+0.7}_{-0.4}  imes 10^{-3}$	1
NH <sub>2</sub> CHO	$5.6^{+1.2}_{-1.1} \times 10^{16}$	[300]	$6.8^{+2.7}_{-1.9} \times 10^{-3}$	1
CH <sub>3</sub> COCH <sub>3</sub>	$1.6^{+0.6}_{-0.5} \times 10^{16}$	$130^{+20}_{-20}$	$2.0^{+1.0}_{-0.7}  imes 10^{-3}$	17
t-HCOOH	$7.7^{+1.1}_{-1.1}  imes 10^{16}$	[300]	$9.5^{+3.4}_{-2.4}  imes 10^{-3}$	1
c-C <sub>2</sub> H <sub>4</sub> O	$5.5^{+0.7}_{-0.5}  imes 10^{15}$	[100]	$6.7^{+2.4}_{-1.5} \times 10^{-4}$	2
c-C <sub>2</sub> H <sub>3</sub> DO	$1.2^{+0.2}_{-0.2} \times 10^{15}$	[100]	$1.5^{+0.5}_{-0.4}  imes 10^{-4}$	2
CH <sub>3</sub> SH	$4.5^{+0.5}_{-0.7} \times 10^{15}$	[100]	$5.5^{+1.9}_{-1.4}  imes 10^{-4}$	2
HOCH <sub>2</sub> 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 ~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 <sup>13</sup>CH<sub>3</sub>OH column density by <sup>12</sup>C/<sup>13</sup>C = 68 (Milam et al. 2005). The FWHM for all molecules is ~1.8 ± 0.5 km s<sup>-1</sup>. 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 (~70%) in the Band 3 spectrum of IRAS16293 B 310 were identified, we could not associate any simple or complex 311 species to ~25 – 30% of lines at the  $\geq 6\sigma$  level. Potentially more 312 high-resolution laboratory spectra are needed to identify those 313 lines. This is particularly important for the (doubly) deuterated 314 isotopologues of known COMs and larger COMs with more than 315 eight atoms. 316

## 3.2. Fitting results for the detected species

Derived column densities and excitation temperatures are given 318 in Table 1. The measured excitation temperatures span a range 319



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  $E_{up}$  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  $E_{up} < 300 \text{ K}$  are shown.

between  $\sim 50$  and  $\sim 300$  K. Figure B.4 presents the excitation 320 temperatures where a determination was possible for molecules 321 with sufficient detected lines. The species on the x-axis are 322 roughly ordered by increasing binding energies in the ice from 323 left to right (Minissale et al. 2022; Ligterink & Minissale 2023). 324 The error bars are too large to robustly confirm whether there is 325 any correlation between the excitation temperature and binding 326 energy. 327

The column densities measured here span a range of ~4 orders of magnitude. The most abundant molecule is methanol, after that (and its isotopologues), CH<sub>3</sub>OCHO and CH<sub>3</sub>OCH<sub>3</sub> 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 CH<sub>3</sub>OH was determined by scaling the <sup>13</sup>CH<sub>3</sub>OH column density by <sup>12</sup>C/<sup>13</sup>C of 68 (Milam et al. 2005) and was found to be  $8.2 \times 10^{18}$  cm<sup>-2</sup> in the ~1" 335 beam. We note that the <sup>13</sup>CH<sub>3</sub>OH lines used for measurement of 336 column density of this molecule are relatively weak and hence 337 optically thin. They either have a large  $E_{up}(\sim 500 \text{ K})$  or a low  $A_{ij}$ 338  $(\sim 6 \times 10^{-8} \text{ s}^{-1})$ . Therefore, <sup>13</sup>CH<sub>3</sub>OH in this study should ro-339 bustly determine the column density of the major isotopologue 340 without the need for  $CH_3^{18}OH$ . The least abundant molecule at 341 the 0.5" offset location is HCCCN with a column density of 342  $6.2 \times 10^{13}$  cm<sup>-2</sup> (see Murillo et al. 2022b for its map). 343

## 3.3. Glycolonitrile and ethylene oxide

Here we focus on the tentative detection of  $HOCH_2CN$  (glycolonitrile) and  $c-C_2H_4O$  (ethylene oxide). These two molecules 346

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 352 lower frequency ( $\leq 266 \,\text{GHz}$ ) observations than PILS (Zeng 353 et al. 2019). Later it was also detected in PILS by Ligterink et al. 354 (2021), mainly toward the half-beam offset position ( $\sim 0.25''$  off-355 set from the continuum peak) and not the full-beam offset po-356 sition (0.5" offset). It is interesting that in the Band 3 data, 357 HOCH<sub>2</sub>CN was tentatively detected toward the full-beam off-358 set position of PILS. This could be due to the larger beam size of 359 the Band 3 observations and the inclusion of the hotter gas close 360 to the protostar in the beam given that the binding energy of this 361 molecule is relatively high (~10400 K; Ligterink & Minissale 362 2023). 363

Our tentative column density ratio of HOCH<sub>2</sub>CN/CH<sub>3</sub>OH 364  $(\sim 10^{-4})$  agrees well with what Ligterink et al. (2021) found 365 for this source in Band 7. Moreover, our column density for 366 367 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) 368 found for their warm component of the same source from their 369 Band 3 data. Moreover, glycolonitrile has been (tentatively) 370 detected toward other objects such as the Serpens SMM1-a 371 protostar and the G+0.693-0.027 molecular cloud with simi-372 lar HOCH<sub>2</sub>CN/CH<sub>3</sub>OH ratios of a few 10<sup>-4</sup> (Requena-Torres 373 374 et al. 2006; Ligterink et al. 2021; Rivilla et al. 2022). A recent 375 study searched for its minor isotopologues in IRAS16293B and 376 SMM1-a, but it resulted in non-detections (Margulès et al. 2023). 377 Ethylene oxide has been detected toward several objects,

mainly high-mass protostars, but also pre-stellar cores and the 378 comet 67P (Dickens et al. 1997; Nummelin et al. 1998; Ikeda 379 et al. 2001; Requena-Torres et al. 2008; Bacmann et al. 2019; 380 Drozdovskava et al. 2019). This molecule has also been detected 381 toward IRAS16293 A and B by PILS (Lykke et al. 2017; Mani-382 gand et al. 2020). The ratio for ethylene oxide to methanol from 383 this work is  $\sim 7 \times 10^{-4}$ , which agrees well with the ratio from 384 PILS of  $\sim 3 - 6 \times 10^{-4}$  (Lykke et al. 2017; Jørgensen et al. 2016, 385 2018). Its deuterated species were studied and detected toward 386 IRAS16293 B by Müller et al. (2023a,b). We also tentatively de-387 388 tected 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 389 data is  $\sim 1 - 2 \times 10^{-4}$  which agrees well with the same ratio in 390 PILS ( $\sim 9 \times 10^{-5}$ ; Jørgensen et al. 2018; Müller et al. 2023a). 391

## 392 4. Discussion

# 393 4.1. Dust optical depth

For this section we calculated the continuum optical depth at ~348.815 GHz (corresponding to ALMA Band 7) and at ~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)

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

where  $F_{\nu}$  is the continuum flux density within the beam,  $\Omega_{\text{beam}} = \pi \theta_{\min} \theta_{\text{maj}} / (4 \ln(2))$  is the beam solid angle with  $\theta_{\min}$  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 ~91 GHz and pink shows the PILS continuum at a frequency of ~348.815 GHz.

found  $F_{\nu}$  to be within the beam of those observations at the peak 404 of the continuum and at the  $\sim 0.5''$  offset position where the spec-405 trum was extracted. For this measurement we used CASA (Mc-406 Mullin et al. 2007) version 6.5.2.26 and found the continuum 407 flux density to be ~1.16 Jy beam<sup>-1</sup> and ~0.55 Jy beam<sup>-1</sup> at the 408 peak and the offset position. We did the same for the Band 3 data 409 at a frequency of ~91 GHz and found the Band 3 continuum flux 410 density to be ~9.07×10<sup>-2</sup> Jy beam<sup>-1</sup> and ~5.25×10<sup>-2</sup> Jy beam<sup>-1</sup> 411 at the peak and the offset positions, respectively. Next, we cal-412 culated  $\tau_{dust}$  for a range of dust temperatures that are feasible for 413 IRAS16293B as suggested by Jacobsen et al. (2018). 414

Figure 4 presents the continuum optical depth for the var-415 ious temperatures. The temperature of the inner regions based 416 on models of Jacobsen et al. (2018) is ~90 K. At 90 K, both the 417 PILS and Band 3 peak continuum are marginally optically thick 418 with the PILS continuum having an optical depth of  $\sim 1.5$  times 419 larger. However, at the location off-source, the dust optical depth 420 for the PILS continuum is almost the same as that of Band 3, 421 which is  $\sim 0.15$ . Therefore, it is safe to assume that the dust at 422 the offset location at  $T_{dust} = 90$  K is almost completely optically 423 thin in Band 3 and Band 7 datasets. Even assuming the unreal-424 istic worst case scenario of  $T_{dust} = 30$  K in Fig. 4 and assuming 425 that all the dust is in a column between the observer and the 426 protostar, the difference between Band 3 and Band 7 dust atten-427 uation (i.e.,  $e^{-\tau}$ ) is around 25% at the offset location at most. 428

## 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. 432

429

433

## 4.2.1. Excitation temperature

The measured excitation temperatures are presented in Fig. B.4. 434 The species are roughly ordered by increasing binding energy (a 435

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

Nevertheless, our excitation temperatures mostly agree with 450 those found by Jørgensen et al. (2018) for IRAS16293 B. The 451 only exceptions are CH<sub>3</sub>OCHO and CH<sub>3</sub>CH<sub>2</sub>OH where their ex-452 citation temperatures are found to be higher in PILS. This could 453 454 be due to the lines that are covered in the Band 3 data having a lower  $E_{up}$  than those covered in the Band 7 data. For example, 455 if the two lines of CH<sub>3</sub>CH<sub>2</sub>OH with  $E_{up} \sim 80 - 90$  K are ignored, 456 a fit at  $T_{\rm ex} \sim 240$  K (i.e., agreeing with the PILS temperature) can 457 match the brightness temperatures of the rest of the lines within 458  $\sim 40 - 50\%$ . Our excitation temperatures also agree well with 459 what is found for the companion source, IRAS16293A, in PILS 460 (Manigand et al. 2020). 461

## 462 4.2.2. Column density

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

Figure 5 presents the column densities from PILS and this 483 work after correction for beam dilution. The column densities of 484 PILS are taken from Coutens et al. (2016) (NH<sub>2</sub>CHO), Jørgensen 485 et al. (2016) (CH<sub>2</sub>OHCHO, CHDOHCHO, gGg-(CH<sub>2</sub>OH)<sub>2</sub>, 486 and CH<sub>3</sub>COOH), Calcutt et al. (2018b) (CH<sub>3</sub>CH<sub>2</sub>CN, HC<sub>3</sub>N), 487 Jørgensen et al. (2018) (CH<sub>3</sub>OH, <sup>13</sup>CH<sub>3</sub>CHO, CH<sub>3</sub>CDO, 488 CH<sub>3</sub>CHO, CH<sub>2</sub>DOH, CH<sub>3</sub>CH<sub>2</sub>OH, a-CH<sub>3</sub>CHDOH, CH<sub>3</sub>OCH<sub>3</sub>, 489 CH<sub>3</sub>OCHO, a-a-CH<sub>2</sub>DCH<sub>2</sub>OH, and t-HCOOH), Persson et al. 490 (2018) (D<sub>2</sub>CO), Manigand et al. (2020) (CH<sub>2</sub>DCHO), Droz-491 dovskaya et al. (2022) (CHD<sub>2</sub>OH), Ilyushin et al. (2022) 492 (CD<sub>3</sub>OH), Drozdovskaya et al. (2018) (CH<sub>3</sub>SH), Ferrer Asen-493 sio et al. (2023) (CHD<sub>2</sub>CHO), and Lykke et al. (2017) 494 (CH<sub>3</sub>COCH<sub>3</sub>). In addition, we did not include <sup>13</sup>CH<sub>2</sub>OHCHO 495 and gGg-(CH<sub>2</sub>OH)<sub>2</sub> in Fig. 5 because our measured column 496



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

densities are approximate. Moreover, the column density of 497 CH<sub>3</sub>COOH in PILS was found from old spectroscopic data 498 (Jørgensen et al. 2016). To avoid a bias, we redid the fit to 499 CH<sub>3</sub>COOH in the Band 7 data using new spectroscopic data 500 (Ilyushin et al. 2013; see Appendix A), and found that the col-501 umn density in Jørgensen et al. (2016) was underestimated by a 502 factor of about two. Therefore, in this work we refer to the up-503 dated column density of CH<sub>3</sub>COOH using the new spectroscopic 504 data (~ $1.2 \times 10^{16}$ ). 505

Figure 5 shows that the column densities from the Band 506 3 observations generally agree with those of PILS. There are 507 a few data points where the Band 3 column densities are  $\gtrsim 3$ 508 times higher than those of Band 7. Among those molecules, 509 NH<sub>2</sub>CHO and CH<sub>3</sub>CH<sub>2</sub>CN seem to be outliers that have Band 510 3 column densities that are ten times higher than Band 7. How-511 ever, because the column densities of these two molecules in this 512 work were measured based on only one line, those values should 513 be considered with caution. Therefore, we excluded these two 514 molecules from further analysis. 515

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

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

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

We found a good match between Band 3 and Band 7 data when comparing the ratios of the various COMs relative to methanol. The molecules that have column densities with a factor of > 2 difference between Band 3 and Band 7 in Fig. 5 (i.e., t-HCOOH, CD<sub>3</sub>OH, and CHD<sub>2</sub>CHO) show good agreement (factor of < 2) when their column density ratios with respect to methanol are compared between the two sets of observations.

## 561 4.3. Comparison with other studies

In this section we put some of the measured ratios (Fig. 2) in the 562 context of other works. We mainly focus on the upper limit ra-563 564 tios because similar comparisons have been made in the PILS papers between the measured column density ratios of IRAS 16293 565 B and other sources. The ratios of aGg'- and gGg'-(CH<sub>2</sub>OH)<sub>2</sub> 566 to CH<sub>3</sub>OH from our observations is between  $\sim 4 \times 10^{-3}$  and 567  $\sim 2 \times 10^{-2}$ . The laboratory experiments and Monte Carlo simula-568 tions found the  $(CH_2OH)_2/CH_3OH$  ratio to be  $\sim 10^{-2} - 9 \times 10^{-2}$ 569 and  $\sim 2 \times 10^{-2} - 4 \times 10^{-2}$  (Fedoseev et al. 2015), which agrees with 570 our observations. Moreover, Fedoseev et al. (2017) found a ratio 571 of glycerol/ethylene glycol upper limit of around 0.01 in labora-572 tory experiments which, from the ethylene glycol/methanol ratio 573 of Fedoseev et al. (2015), gives a glycerol/methanol upper limit 574 of between  $10^{-4}$  and  $9 \times 10^{-4}$ . Our upper limit ratios of GGag'g'-575 and G'Gg'gg'-glycerol to methanol are  $<10^{-4}$  and  $<8 \times 10^{-4}$ . 576 which are on the same order of magnitude as reported in labora-577 tory experiments and Monte Carlo simulations (Fedoseev et al. 578 2015, 2017). 579

Propanal was found to form n-propanol (Qasim et al. 2019a,b), and both were not detected in the Band 3 data. However, we note that propanal was detected toward IRAS 16293 B by PILS (Lykke et al. 2017) and Qasim et al. (2019a) found that the ratio of their upper limit ratio for n-propanol/propanal for 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  $<7 \times 10^{-4}$ , 586 which is a factor of about six lower than the detected ratio to-587 ward G+0.693-0.027 ( $\sim 4 \times 10^{-3}$ ; Jiménez-Serra et al. 2022 and 588 methanol from Rodríguez-Almeida et al. 2021). Our upper limit 589 ratios of g-, a-Isopropanol, and Ga-n-propanol with respect to 590 methanol agree within a factor of about two with those detected 591 toward Sgr B2(N2b) (~0.002; Belloche et al. 2022). Band 3 ra-592 tios of s- and g-propanal/methanol are  $< 2 \times 10^{-4}$  and < 0.04, re-593 spectively. These are in agreement with the abundance ratios of 594 propanal/methanol in TMC-1 (around 0.01, Agúndez et al. 2023) 595 and PILS (around  $2 \times 10^{-4}$ ; Lykke et al. 2017). Moreover, the 596 abundance of indene with respect to H<sub>2</sub> toward TMC-1 (Cer-597 nicharo et al. 2021) is on the same order of magnitude as our 598 upper limit ratio of indene/H<sub>2</sub>, assuming a lower limit on the 599  $H_2$  column density of  $10^{25}$  cm<sup>-2</sup> from Jørgensen et al. (2016) 600 for IRAS 16293 B. However, using the same lower limit col-601 umn density for H<sub>2</sub> toward IRAS 16293 B, our upper limit abun-602 dances of 1-CNN, 2-CNN, and benzonitrile are a factor of about 603 two to ten lower than what is found for TMC-1 (Gratier et al. 604 2016: McGuire et al. 2021). 605

The Band 3 upper limit ratio of urea/methanol is  $< 2 \times 10^{-5}$ , 606 which is in-line and on the lower end of the observed range 607 (either upper limit or detected) in the literature toward SgrB2 608 (Belloche et al. 2019), NGC 6334I (Ligterink et al. 2020), and 609 G+0.693-0.027 systems (Zeng et al. 2023). The upper limit 610 NH<sup>13</sup>CHO/CH<sub>3</sub>OH in this work is consistent with the detected 611 ratios toward NGC 6334I (Ligterink et al. 2020; methanol from 612 Bøgelund et al. 2018) and G+0.693-0.027 systems (Zeng et al. 613 2023; methanol from Rodríguez-Almeida et al. 2021). More-614 over, the upper limit ratios of z-cyanomethanimine and glyc-615 eraldehyde to methanol toward G+0.693-0.027 (Jiménez-Serra 616 et al. 2020) are consistent with our upper limit ratios. However, 617 the ratio of ethanolamine/methanol toward this source (Rivilla 618 et al. 2021) was found to be around one order of magnitude 619 higher than the Band 3 upper limit measurement of IRAS 16293 620

B. The discussed ratios in this section may be generally higher 621 in G+0.693-0.027 than IRAS 16293 B. Given the small sample 622 size and the upper limit nature of our results, it is not possible to 623 draw further conclusions on the significance of these differences 624 and similarities. This is particularly the case, because of the up-625 per limits reported here tend to depend on the assumed excitation 626 temperature and more importantly the lines covered in our data. 627

#### 5. Conclusions 628

We analyzed the deep ALMA Band 3 (~100 GHz) data of 629 IRAS16293 B in this work. We searched for large organic 630 species in this dataset and derived the corresponding col-631 umn densities and excitation temperatures of various oxygen-632 , nitrogen-, and sulfur-bearing molecules. Below are the main 633 conclusions of this work. 634

- The line density for lines detected at a  $\gtrsim 6\sigma$  level in Band 3 635 observations is one per ~8.5 MHz, which is only ~2.5 times 636 lower than that of PILS: the spectrum is relatively rich and 637 crowded even at ~3 mm observations. 638
- We detected around 31 molecules (including minor isotopo-639 logues), thereof ~15 tentatively, in the Band 3 dataset. These 640 include O-bearing COMs such as CH<sub>3</sub>OH, CH<sub>2</sub>OHCHO, 641 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 642 c-C<sub>2</sub>H<sub>4</sub>O. We also tentatively detected a few N- and S-643 bearing species such as HOCH<sub>2</sub>CN and CH<sub>3</sub>SH. 644
- We searched for many large COMs among which are glyc-645 erol and isopropanol, but we did not detect them. The up-646 per limits on the 41 non-detected species are also provided, 647 which generally agree with the previous laboratory experi-648 ments and observations. 649
- In the Band 3 spectrum,  $\sim 25 30\%$  of all lines at the  $\gtrsim 6\sigma$ 650 level were not identified. This points to the need for addi-651 tional spectroscopic information. 652
- We find good agreement between the column densities of 653 Band 3 and Band 7 observations with a scatter of less than 654 a factor of two. Moreover, the Band 3 ratios with respect to 655 methanol agree within a factor of about two with those from 656 the Band 7 observations. 657
- We conclude that around IRAS16293 B, the dust optical 658 depth does not affect the column densities and the ratios 659 of various molecules, especially for the spectrum extracted 660 from a position off-source (where the dust column density is 661 662 lower than on-source).
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## Table A.1: Spectroscopic information

Name	Species	Catalog	References
Methanol	<sup>13</sup> CH <sub>3</sub> OH	CDMS	Xu & Lovas (1997)
Methanol	CH <sub>2</sub> DOH	JPL	Pearson et al. (2012)
Methanol	CHD <sub>2</sub> OH	CDMS	Drozdovskaya et al. (2022)
Methanol	CD <sub>3</sub> OH	CDMS	Ilyushin et al. (2022)
Acetaldehyde	CH <sub>3</sub> CHO	JPL	Kleiner et al. (1996)
Acetaldehyde	<sup>13</sup> CH <sub>3</sub> CHO	CDMS	Margulès et al. (2015)
Acetaldehyde	CH <sub>2</sub> DCHO	CDMS	Coudert et al. (2019)
Acetaldehyde	CH <sub>3</sub> CDO	CDMS	Coudert et al. (2019)
Acetaldehyde	CHD <sub>2</sub> CHO	JPL format	Ferrer Asensio et al. (2023)
Acetic acid	CH <sub>3</sub> COOH	CDMS	Ilyushin et al. (2013)
Glycolaldehyde	CH <sub>2</sub> OHCHO	CDMS	Müller 2021, unpublished
Glycolaldehyde	13CH2OHCHO	CDMS	Haykal et al. (2013)
Glycolaldehyde	CHDOHCHO	CDMS	Bouchez et al. (2012)
Ethanol	CH <sub>3</sub> CH <sub>2</sub> OH	CDMS	Pearson et al. (2008); Müller et al. (2016)
Ethanol	a-a-CH2DCH2OH	CDMS	Walters et al. (2015)
Ethanol	a-CH <sub>3</sub> CHDOH	CDMS	Walters et al. (2015)
Dimethyl ether	CH <sub>3</sub> OCH <sub>3</sub>	CDMS	Endres et al. (2009)
Methyl formate	CH <sub>3</sub> OCHO	JPL	Ilyushin et al. (2009)
aGg'-ethylene glycol	aGg'-(CH2OH)2	CDMS	Christen et al. (1995); Christen & Müller (2003)
gGg'-ethylene glycol	gGg'-(CH2OH)2	CDMS	Christen et al. (2001); Müller & Christen (2004)
Formaldehyde	D <sub>2</sub> 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	CH <sub>3</sub> CH <sub>2</sub> CN	CDMS	Pearson et al. 1994; Fukuyama et al. 1996;
			Brauer et al. 2009
Formamide	NH <sub>2</sub> CHO	CDMS	Kukolich & Nelson 1971; Hirota et al. 1974;
			Kryvda et al. 2009; Motiyenko et al. 2012
Acetone	CH <sub>3</sub> COCH <sub>3</sub>	JPL	Groner et al. (2002); Ordu et al. (2019)
Formic acid	t-HCOOH	CDMS	Winnewisser et al. (2002)
Ethylene oxide	c-C <sub>2</sub> H <sub>4</sub> O	CDMS	Creswell & Schwendeman (1974); Hirose (1974);
			Medcraft et al. (2012)
Ethylene oxide	c-C2H3DO	CDMS	Müller et al. (2023a)
Methanethiol	CH <sub>3</sub> SH	CDMS	Zakharenko et al. (2019)
Glycolonitrile	HOCH <sub>2</sub> 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).

## 964 Appendix A: Spectroscopic data

The spectroscopic information are summarized in Table A.1. 965 The vibrational correction factor is assumed as one for all 966 molecules except for the following species. The vibrational 967 correction factor of 1.457 was used for CH2DOH at a tem-968 perature of 300 K (Lauvergnat et al. 2009; Jørgensen et al. 969 2018). For CH<sub>2</sub>OHCHO, a factor of 2.86 was adopted at 300K 970 to take the higher (than ground state) vibrational states into 971 account, which were calculated in the harmonic approxima-972 tion. For <sup>13</sup>CH<sub>2</sub>OHCHO and CHDOHCHO, a vibrational fac-973 tor of 2.8 was used at a temperature of 300 K (Jørgensen et al. 974 2016). An upper limit vibrational factor of 2.824 at 300 K 975 (Durig et al. 1975; Jørgensen et al. 2018) was assumed for a-976 a-CH<sub>2</sub>DCH<sub>2</sub>OH and a-CH<sub>3</sub>CHDOH. Moreover, following Jør-977 gensen et al. (2018), we multiplied the column densities of these 978 two species by an additional factor of  $\sim 2.69$  to account for the 979 presence of the gauche conformer. We assumed a vibration cor-980 rection factor of 4.02 for aGg-(CH<sub>2</sub>OH)<sub>2</sub> and gGg-(CH<sub>2</sub>OH)<sub>2</sub> 981 and added an additional factor of ~1.38 to include the contribu-982 tion from the higher gGg conformer at 300 K (Müller & Christen 983 2004; Jørgensen et al. 2016). A vibrational correction factor of 984 1.09 at 100 K was used for HCCCN (Mallinson & Fayt 1976; 985 Calcutt et al. 2018b). For CH<sub>3</sub>CH<sub>2</sub>CN, a vibrational correction 986 factor of 1.113 was assumed at 100 K. A vibrational correction 987 factor of 1.5 was assumed for NH<sub>2</sub>CHO at 300 K. For t-HCOOH, 988 a vibrational correction factor of 1.103 at 300 K was assumed 989 (Perrin et al. 2002; Baskakov et al. 2006; Jørgensen et al. 2018). 990

## Appendix B: Additional plots and tables

Figure **B**.1 presents the fitted models of each molecule to the 992 Band 3 data, highlighting a number of lines that are yet to be 993 determined. Figures B.2 and B.3 present the transitions of Ga-994 n-propanol and G'Gg'gg'-Glycerol with the models determining 995 their upper limits in orange. The total fit to the detected and ten-996 tative molecules is also shown in cyan. Figure B.4 presents the 997 excitation temperatures when a measurement was possible for 998 Band 3 results (PILS temperatures are shown for comparison). 999 Figure B.5 shows the comparison of Band 3 and Band 7 beams 1000 on top of a two-dimensional Gaussian distribution, representing 1001 the spatial extents of COMs (e.g., see Jørgensen et al. 2016). 1002 This was done to examine the difference between the mean flux 1003 in the two beams, which is around 10%. Table B.1 shows the up- 1004 per limits found for the molecules searched for but not detected. 1005 Table B.2 presents the covered transitions of the (tentatively) de- 1006 tected molecules in the data. 1007



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  $aGg'-(CH_2OH)_2$ , which are potentially optically thick. The lines that have an intensity higher than 2 K (i.e., detected at a  $\gtrsim 7 - 10\sigma$  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  $300 \pm 60$  K or  $125 \pm 25$  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.

Name	Molecular formula	Upper limit (cm <sup>-2</sup> )
Methanol	CH <sup>18</sup> OH	<5.0×10 <sup>17</sup>
Formamide	NH <sub>2</sub> CDO	<2.0 ×10 <sup>15</sup>
Formamide	NH <sup>13</sup> CHO	<1.2 ×10 <sup>16</sup>
Formamide	cis-NHDCHO	<2.5 ×10 <sup>15</sup>
Formamide	trans-NHDCHO	<5.0×10 <sup>15</sup>
Formamide	$NH_2CHO(v_{12} = 1)$	<5.0×10 <sup>17</sup>
Z-cyanomethanimine	Z-HNCHCN	<5.5 ×10 <sup>15</sup>
Methanethiol	<sup>13</sup> CH <sub>3</sub> SH	$<7.0 \times 10^{15}$
Cyanodiacetylene	HC <sub>5</sub> N	$<2.0 \times 10^{13}$
Ethylene oxide	c-CD <sub>2</sub> CH <sub>2</sub> O	<6.0 ×10 <sup>14</sup>
Acetaldehyde	CH <sub>2</sub> <sup>13</sup> CHO	$< 6.0 \times 10^{15}$
Vinyl cyanide	C <sub>2</sub> H <sub>3</sub> CN	$<4.0 \times 10^{15}$
Glycolaldehyde	CH <sub>2</sub> OHCDO	$< 1.0 \times 10^{15}$
Glycolaldehyde	CH <sub>2</sub> ODCHO	$< 5.0 \times 10^{14}$
Glycolaldehyde	CH <sub>2</sub> OH <sup>13</sup> CHO	$< 1.5 \times 10^{15}$
Methyl formate	CH <sub>3</sub> O <sup>13</sup> CHO	$<7.0 \times 10^{15}$
Propargyl cyanide	HCCCH <sub>2</sub> CN	$<7.0 \times 10^{14}$
Propenal	C <sub>2</sub> H <sub>3</sub> CHO	$< 1.5 \times 10^{14}$
Protonated cyanodiacetylene	HC <sub>5</sub> NH <sup>+</sup>	$< 1.5 \times 10^{13}$
Urea	H <sub>2</sub> NCONH <sub>2</sub>	$< 1.5 \times 10^{14}$
Ethanol	a-13CH3CH2OH	$< 8.0 \times 10^{14}$
Ethanol	a-CH <sub>3</sub> <sup>13</sup> CH <sub>2</sub> OH	$< 1.5 \times 10^{18}$
Ethanol	a-CH <sub>3</sub> CH <sub>2</sub> OD	$< 1.0 \times 10^{15}$
Ethanol	a-s-CH2DCH2OH	$<3.0 \times 10^{15}$
Gauche-ethyl mercaptan	g-C <sub>2</sub> H <sub>5</sub> SH	$< 1.0 \times 10^{15}$
Methoxymethanol	CH <sub>3</sub> OCH <sub>2</sub> OH	$< 4.0 \times 10^{17}$
s-propanal	s-C <sub>2</sub> H <sub>5</sub> CHO	$< 1.5 \times 10^{15}$
g-propanal	g-C <sub>2</sub> H <sub>5</sub> CHO	$<3.5 \times 10^{17}$
Cyclopentadiene	c-C <sub>5</sub> H <sub>6</sub>	$< 5.0 \times 10^{16}$
Ethanolamine	NH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> OH	$< 6.0 \times 10^{14}$
Ga-n-propanol	Ga-n-C <sub>3</sub> H <sub>7</sub> OH	$< 6.0 \times 10^{15}$
Glyceraldehyde	HCOCHOHCH <sub>2</sub> OH	$< 8.0 \times 10^{15}$
g-Isopropanol	g-i-C <sub>3</sub> H <sub>7</sub> OH	$< 1.5 \times 10^{16}$
a-Isopropanol	a-i-C <sub>3</sub> H <sub>7</sub> OH	$<2.0 \times 10^{16}$
Benzonitrile	c-C <sub>6</sub> H <sub>5</sub> CN	$< 1.0 \times 10^{14}$
Benzaldehyde	c-C <sub>6</sub> H <sub>5</sub> CHO	$<7.0 \times 10^{14}$
GGag'g'-Glycerol	GGag'g'-HOCH <sub>2</sub> CH(OH)CH <sub>2</sub> OH	$<\!8.0 imes\!10^{14}$
G'Gg'gg'-Glycerol	G'Gg'gg'-HOCH <sub>2</sub> CH(OH)CH <sub>2</sub> OH	$<7.0 \times 10^{15}$
Indene	c-C9H8	$< 1.0 \times 10^{16}$
1-cyanonaphthalene	1-C <sub>10</sub> H <sub>7</sub> CN	$< 1.0 \times 10^{14}$
2-cyanonaphthalene	2-C <sub>10</sub> H <sub>7</sub> CN	$<\!\!2.0  imes 10^{14}$

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

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

	Treeseitier	<b>E</b>	4	F
Species		Frequency	$A_{ij}$	$E_{\rm up}$
	J K L M	(MHZ)	$\frac{(s^{-1})}{200 + 10-6}$	(K)
CH <sub>3</sub> OH	20 3 18 5 - 19 2 18 5	90813.078	$2.80 \times 10^{-6}$	808.3
	20 2 18 2 - 20 2 19 1	91 254.751	$5.29 \times 10^{-6}$	514.3
	1014-2124	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	90762.771	$5.43 \times 10^{-8}$	580.9
	2110-1100	90779.841	$1.57 \times 10^{-6}$	10.6
	25 0 25 1 - 24 3 21 2	91 043.068	$2.77 \times 10^{-7}$	702.0
	9181-9091	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	10321-11021	90701.939	$5.61 \times 10^{-8}$	144.1
- 2 -	20 4 1 1 - 20 4 2 0	90717.394	$1.02 \times 10^{-9}$	474.9
	18 4 2 0 - 18 3 1 2	90737.495	$7.34 \times 10^{-7}$	392.4
	10 4 2 1 - 11 3 2 0	90756.808	$4.52 \times 10^{-7}$	165.0
	10212-9312	90757.511	$5.45 \times 10^{-7}$	141.1
	2112-3111	90767.952	$1.35 \times 10^{-9}$	27.7
	8210-8021	90 863.187	$3.73 \times 10^{-9}$	84.9
	6212-7210	90 945.187	$1.94 \times 10^{-9}$	73.2
	12012-12220	90 972.887	$6.69 \times 10^{-9}$	173.9
	10411-11310	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
	6122-7120	103 504.343	$3.22 \times 10^{-9}$	63.3
CD <sub>3</sub> OH	10461-11381	103 298.627	$1.47 \times 10^{-6}$	156.5
CH <sub>3</sub> CHO	25 3 23 3 - 26 0 26 3	90618.941	$2.12 \times 10^{-8}$	526.0
	7354-8274	90 622.765	$5.86 \times 10^{-7}$	250.3
	4231-5052	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	90723.537	$1.86 \times 10^{-8}$	636.9
	31 2 29 0 - 32 0 32 0	90730.219	$2.82 \times 10^{-9}$	475.7
	13 2 11 6 - 14 1 14 6	90731.485	$6.83 \times 10^{-7}$	471.1
	37 4 33 5 - 37 4 34 4	90737.826	$3.52 \times 10^{-7}$	897.9
	21 6 15 5 - 22 5 17 5	90743.918	$6.78 \times 10^{-7}$	500.7
	35 4 32 4 - 36 2 35 4	90746.919	$3.37 \times 10^{-9}$	825.9
	29 3 27 4 - 29 2 27 5	90791.888	$1.23 \times 10^{-9}$	628.4
	21 2 19 6 - 22 1 22 6	90 856.686	$3.05 \times 10^{-7}$	604.1
	9095-8175	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
	5058-4048	90910.33	$2.42 \times 10^{-5}$	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	$5.97  imes 10^{-7}$	355.3

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

Table B.2:	continued.
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$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$	Species	Transition	Frequency	$A_{ij}$	$E_{\rm up}$
$ \begin{array}{c} 3.03 \ . 28 \ . 7 \ . 10 \ . 88.24 \ . 3.10 \ . 10^{-9} \ . 88.93 \ . 3.10 \ . 10^{-9} \ . 73.4 \ . 10^{-7} \ . 73.4 \ . 10^{-7} \ . 10.5 \ . 10^{-7}$		J K L M 20.2.29.7 21.0.21.9	(MHZ)	$\frac{(s^{-1})}{5.00 \times 10^{-9}}$	(K)
$ \begin{array}{c} 111100 - 110110 & 91188.22 & 3.22 \times 10^{-1} & 64.8 \\ 36 \times 33 \times 37 \times 10^{-9} & 733 \\ 31 \times 10^{-9} & 733 \\ 31 \times 10^{-9} & 734 \\ 32 \times 10^{-7} & 731 \\ 33 \times 30 & 1 \times 32 & 331 \\ 103 \times 10^{-8} & 10^{-7} & 516.1 \\ 33 \times 30 & 1 \times 32 & 331 \\ 103 \times 10^{-8} & 10^{-7} & 516.1 \\ 33 \times 30 & 1 \times 32 & 320 \\ 32 \times 10^{-2} & 23 \times 20 \\ 32 \times 10^{-2} & 23 \times 20 \\ 32 \times 10^{-3} & 335 \\ 30 \times 23 \times 31^{-7} & 23 \\ 30 \times 22 \times 31^{-7} & 23 \\ 30 \times 30^{-5} & 7.34 \times 10^{-7} \\ 30 \times 22 \times 31^{-7} & 23 \\ 30 \times 30^{-5} & 7.34 \times 10^{-7} \\ 30 \times 10^{-7} & 7194 \\ 30 \times 22 \times 31^{-7} & 23 \\ 30 \times 30^{-7} & 734 \times 10^{-7} \\ 30 \times 10^{-7} & 7194 \\ 31 \times 43 \times 43 \times 31^{-3} & 30 \\ 31 \times 10^{-7} & 7194 \\ 31 \times 43 \times 41^{-3} & 32 \times 21^{-3} & 910520^{-7} & 734 \times 10^{-7} \\ 31 \times 10^{-8} & 7164 \\ 51 5 \times 1^{-4} 14 \times 3 \\ 90 9035.753 & 241 \times 10^{-5} & 154 \\ 51 5 \times 1^{-4} 14 \times 3 \\ 90 9051.18 & 2.41 \times 10^{-5} & 154 \\ 31 \times 43 \times 41^{-3} & 32 \times 21^{-3} & 910520^{-7} & 734 \times 10^{-7} \\ 225 \times 23 \times 3^{-3} & 20 \times 23^{-7} & 39130^{-8} \\ 31 \times 10^{-7} & 7252 \\ 22 \times 32 \times 3^{-3} & 20 \times 31^{-7} & 3134 \times 10^{-7} & 7253 \\ 32 \times 28 \times 10^{-3} & 332 \times 30^{-7} & 103333.904 \\ 51 5 \times 1^{-4} 14 \times 31^{-7} & 91388 \\ 31 \times 10^{-7} & 7253 \\ 32 \times 28 \times 10^{-3} & 3310 \times 10^{-7} & 3254 \\ 310 \times 10^{-7} & 3254 $		30 3 28 / - 31 0 31 8	91 155.32	$5.90 \times 10^{-6}$	829.2
$ \begin{array}{c} 304 4.34 - 35 2.344 & 91 183.824 & 3.10 \times 10^{-1} 923.4 \\ 315 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 \\ 52 4 7 - 41 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 - 35 234 1 & 103 378.41 & 1.03 \times 10^{-8} 587.9 \\ 32 2 30 5 - 33 0 33 5 & 103 345.991 & 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 - 111 10 3 & 103 456.903 & 4.86 \times 10^{-9} 77.94 \\ 30 8 22 3 - 31 7 22 3 & 103 496.344 & 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 \\ 30 8 22 3 - 31 7 25 3 & 103 496.344 & 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 \\ 1^{3} CH_{3} CHO & 37 6 32 - 3 67 29 - 3 & 90 765.097 & 7.39 \times 10^{-7} 655.2 \\ 22 3 20 - 3 - 28 6 22 - 3 & 90 791.095 & 7.33 \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 9051.18 & 2.41 \times 10^{-5} 15.4 \\ 5 1 5 5 1 - 4 1 4 1 & 90 9051.18 & 2.41 \times 10^{-5} 15.4 \\ 33 4 30 - 3 - 34 2 33 - 3 & 90 9061.839 & 1.73 \times 10^{-8} 746.1 \\ 5 1 5 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 2 7 - 2 - 28 4 24 - 2 & 91 172.915 & 1.78 \times 10^{-8} 612.2 \\ 25 3 23 - 26 0 2 - 3 0 2 37 - 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 \\ 32 5 2 5 0 - 31 6 2 5 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} 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 & 897 \times 10^{-9} 758.9 \\ 36 9 27 - 3 - 37 8 29 - 3 & 93 187.007 & 8.16 \times 10^{-8} 378.7 \\ 18 3 16 - 3 - 19 0 1 - 3 & 103 335.904 & 2.05 \times 10^{-8} 943.5 \\ 18 3 16 - 3 - 19 0 1 - 3 & 103 335.904 & 2.05 \times 10^{-8} 943.5 \\ 18 3 16 - 3 - 19 0 19 - 3 & 103 335.904 & 2.05 \times 10^{-8} 3$		11 1 10 0 - 11 0 11 0	91 188.823	$3.22 \times 10^{\circ}$	04.8 850.2
$\begin{array}{c} 314 + 314 + 32 + 34 + 32 + 4 & 91 + 21, 169 & 5.75 \times 10^{-7} & 7561.\\ 201 + 198 + 193 + 177 & 93 + 202, 965 & 6.38 \times 10^{-9} & 581.\\ 334 + 301 + 34 + 233 & 103 + 321.687 & 1.06 \times 10^{-8} & 556.4 \\ 52 + 47 - 41 + 138 & 103 + 268.7 & 103 + 276 \times 10^{-8} & 556.4 \\ 34 + 431 + -35 + 234 & 103 + 236.134 & 1.05 \times 10^{-8} & 587.9 \\ 34 + 311 + 35 + 234 & 103 + 378.41 & 1.03 \times 10^{-8} & 587.9 \\ 32 + 230 5 - 330 + 335 + 1 & 103 + 378.41 & 1.03 \times 10^{-8} & 587.9 \\ 32 + 230 5 - 330 + 335 + 1 & 103 + 395.991 & 3.64 \times 10^{-9} & 711.1 \\ 36 + 532 1 - 37 + 335 + 1 & 103 + 436.903 & 486 \times 10^{-6} & 674.0 \\ 11 + 29 + 111 + 103 & 103 + 456.903 & 486 \times 10^{-6} & 779.9 \\ 30 + 22 + 3 - 111 + 103 & 103 + 456.903 & 486 \times 10^{-7} & 779.4 \\ 30 + 22 + 3 - 121 + 23 + 23 + 103 + 436.903 & 486 \times 10^{-7} & 779.4 \\ 30 + 22 + 3 - 23 + 22 + 3 & 29 + 976.5097 & 7.94 \times 10^{-7} & 779.4 \\ 30 + 22 + 3 - 23 + 22 + 3 & 29 + 976.5097 & 7.94 \times 10^{-7} & 765.2 \\ 16 + 21 + 1 - 15 + 12 + 1 & 99 + 990 + 2.2 & 692 \times 10^{-8} & 132.8 \\ 27 + 72 - 3 - 28 + 62 + 3 & 90 + 983.0059 & -7.34 \times 10^{-7} & 655.2 \\ 22 + 3 20 + 3 - 23 + 0 + 23 + 3 & 91 + 990 + 1.18 & 2.41 \times 10^{-5} & 15.4 \\ 31 + 30 + 3 - 34 + 23 + 3 & 91 + 90 + 51.18 & 2.41 \times 10^{-5} & 15.4 \\ 31 + 3 - 35 + 23 + 3 & 91 + 90 + 51.18 & 2.41 \times 10^{-5} & 15.4 \\ 31 + 3 - 35 + 23 + 3 & 91 + 91 + 32 + 10^{-5} & 15.4 \\ 29 + 22 + 7 - 2 + 8 + 24 + 2 & 91 + 172.915 & 1.78 \times 10^{-8} & 716.8 \\ 29 + 22 + 7 - 2 + 8 + 24 + 2 & 91 + 172.915 & 1.78 \times 10^{-8} & 612.2 \\ 25 + 23 + 3 - 37 + 23 + 3 & 91 + 313.98 & 3.30 \times 10^{-8} & 253.5 \\ 32 + 2 + 1 - 4 + 2 + 1 & 91 + 30 + 232.8 & 33 + 10^{-7} & 251.6 \\ 11 + 1 + 0 - 2 + 1 + 1 + 0 - 2 + 13 + 30 + 10^{-7} & 252.5 \\ 22 + 1 - 4 + 2 + 1 & 91 + 313.9 + 30 + 20 \times 10^{-7} & 252.5 \\ C + 3 + 1 + 3 + 19 + 19 + 3 + 13 + 30 + 10^{-8} & 51.6 \\ 11 + 1 - 15 + 12 + 14 + 30 + 2073, 736 & 2.41 \times 10^{-7} & 315.3 \\ 12 + 1 + 4 + 3 + 12 + 91 + 143 + 30 + 2073, 736 & 2.41 \times 10^{-7} & 315.3 \\ 22 + 1 + 4 + 2 + 2 + 1 + 103 + 300, 733 + 91 + 10.7 & 539.8 \\ 16 + 1 - 15 + 13 + 4 & 103 + 103 + 300.73 & 9$		30 4 33 4 - 37 2 30 4	91 189.824	$3.10 \times 10^{-9}$	839.5
$ \begin{array}{c} 313\ 27\ 0 - 30\ 624\ 0 & 91\ 290\ 802\ 2 & 77\ 10\ 10\ 8\ 10\ 31\ 63\ 10\ 7\ 9\ 85\ 11\ 33\ 4\ 30\ 1 - 34\ 2\ 33\ 1 & 10\ 33\ 20\ 20\ 63\ 8\ 10\ 10\ 8\ 55\ 63\ 11\ 0\ 9\ 8\ 55\ 10\ 7\ 520\ 8\ 55\ 10\ 7\ 520\ 8\ 55\ 10\ 7\ 520\ 8\ 55\ 10\ 7\ 75\ 11\ 10\ 33\ 22\ 30\ 5\ 32\ 10\ 33\ 50\ 8\ 10\ 33\ 54\ 8\ 10\ 10\ 7\ 779\ 40\ 15\ 50\ 51\ 10\ 10\ 7\ 779\ 40\ 15\ 50\ 51\ 10\ 10\ 7\ 779\ 40\ 11\ 10\ 3\ 32\ 6\ 50\ 9\ 10\ 50\ 7\ 779\ 40\ 11\ 10\ 3\ 32\ 50\ 50\ 9\ 10\ 10\ 7\ 779\ 40\ 11\ 10\ 3\ 32\ 50\ 50\ 9\ 10\ 10\ 7\ 779\ 40\ 11\ 10\ 3\ 10\ 3\ 45\ 6\ 50\ 9\ 0\ 10\ 7\ 779\ 40\ 11\ 10\ 3\ 10\ 3\ 45\ 6\ 50\ 9\ 0\ 10\ 7\ 779\ 40\ 11\ 10\ 3\ 10\ 3\ 45\ 6\ 50\ 9\ 0\ 10\ 7\ 779\ 40\ 11\ 10\ 3\ 10\ 3\ 45\ 6\ 50\ 9\ 0\ 10\ 7\ 779\ 40\ 11\ 10\ 3\ 10\ 3\ 45\ 6\ 50\ 9\ 0\ 10\ 7\ 779\ 40\ 11\ 10\ 3\ 10\ 3\ 45\ 6\ 50\ 9\ 0\ 10\ 7\ 779\ 40\ 11\ 10\ 3\ 10\ 3\ 45\ 6\ 10\ 10\ 7\ 779\ 40\ 11\ 10\ 3\ 10\ 10\ 10\ 10\ 10\ 10\ 10\ 10\ 10\ 10$		34 4 31 4 - 35 2 34 4	91 215.789	$3.73 \times 10^{-7}$	795.4 516.1
$\begin{array}{c c c c c c c c c c c c c c c c c c c $		31 5 27 0 - 30 6 24 0	91 290.802	$7.77 \times 10^{-9}$	501 1
$\begin{array}{c} 53.4 + 30.1 - 34.2 + 33.1 \\ 52.4 - 4.1 + 38 \\ 53.2 + 20.5 - 32.3 + 20 \\ 33.2 + 20.5 - 33.0 + 30.3 + 2.35 + 4.1 + 103 + 10^{-7} \\ 520.8 \\ 34.4 + 31 + 35.2 + 34.1 \\ 34.4 + 31 + 35.2 + 34.1 \\ 34.4 + 31 + 35.2 + 34.1 \\ 36.5 + 21 + 37.3 + 35.1 \\ 36.5 + 21 + 37.3 + 35.1 \\ 36.5 + 22 + 37.3 + 35.1 \\ 36.5 + 22 + 37.3 + 35.1 \\ 30.8 + 22.0 + 37.3 + 103 + 36.6 + 10^{-7} \\ 30.8 + 22.3 + 31.7 + 24.3 \\ 30.8 + 22.3 + 31.7 + 24.3 \\ 30.8 + 22.3 + 31.7 + 24.3 \\ 30.8 + 22.3 + 31.7 + 24.3 \\ 30.8 + 22.3 + 31.7 + 24.3 \\ 30.8 + 22.3 + 31.7 + 24.3 \\ 30.8 + 22.3 + 31.7 + 24.3 \\ 30.8 + 22.3 + 31.7 + 24.3 \\ 30.8 + 22.3 + 31.7 + 24.3 \\ 30.8 + 22.3 + 31.7 + 24.3 \\ 30.8 + 22.3 + 31.7 + 24.3 \\ 30.8 + 22.3 + 31.7 + 24.3 \\ 30.8 + 22.3 + 31.7 + 24.3 \\ 30.8 + 22.3 + 30.7 + 24.4 \\ 30.7 + 20.3 + 26.2 + 2.3 \\ 90.7 + 10.9 + 7.3 + 4.10^{-7} \\ 91.8 + 22.4 \\ 27.7 + 20.3 + 28.6 + 22.3 & 90.7 + 50.5 \\ 22.3 + 20.3 - 23.0 + 23.3 & 90.9 + 04.355 \\ 22.5 + 20.3 - 23.0 + 23.3 & 30.9 + 00.4 + 52.6 \\ 51.5 + 4.1 + 4.0 \\ 90.9 + 57.5 + 24.4 + 10^{-5} \\ 1.5 + 4.1 + 4.1 \\ 90.9 + 51.18 + 2.4 + 10^{-5} \\ 1.5 + 4.1 + 4.3 \\ 91.9 + 51.18 + 2.4 + 10^{-5} \\ 1.5 + 4.4 + 4.1 + 30.9 + 51.18 + 10^{-8} \\ 51.5 + 3.4 + 4.4 + 3.9 + 1058.163 \\ 1.68 + 10^{-8} \\ 77.68 \\ 22.2 + 2.2 + 28.4 + 2.9 \\ 91.7 + 10.5 + 10.7 + 10.6 \\ 11.2 + 2.2 + 2.1 \\ 23.2 + 2.2 + 2.1 \\ 91.3 + 2.9 + 10.7 + 20.5 \\ 23.1 + 2.2 + 1.9 + 130.5 + 22 + 10.1 \times 10^{-7} \\ 23.5 \\ 32.5 + 2.0 + 3.1 + 2.2 + 1.9 + 130.5 + 2.1 \\ 34.4 + 31 - 3.5 + 2.4 + 2.9 \\ 10.1 + 20^{-7} \\ 22.5 + 2.3 + 2.3 + 2.3 + 2.3 \\ 91.9 + 30.5 + 2.9 + 10.0 + 10^{-7} \\ 22.5 + 2.3 + 2.3 + 2.3 + 2.3 \\ 91.9 + 30.5 + 2.2 + 10.1 \times 10^{-7} \\ 98.5 + 2.2 + 2.2 + 2.1 \\ 91.3 + 2.0 + 3.1 + 10^{-7} \\ 93.5 + 2.4 + 2.3 + 2.3 + 2.3 \\ 91.9 + 30.5 + 2.2 + 10.1 \times 10^{-7} \\ 93.5 + 2.4 + 2.3 + 2.3 + 2.3 \\ 91.9 + 30.5 + 2.2 + 2.1 \\ 91.9 + 30.5 + 2.2 + 2.1 \\ 91.9 + 30.5 + 2.2 + 2.1 \\ 91.9 + 30.5 + 2.2 + 2.1 \\ 91.9 + 30.5 + 2.2 + 2.1 \\ 91.9 + 30.5 + 2.2 + 2.1 \\ 91.9 + 30.5 + 2.2 + 2.1 \\ 91.9 + 30.5 + 2.2 + 2.1 \\ 91.9 + 30.5 + 2.2 + 2.1 \\ 91.9 + 30.5 + 2.2 + 2.1 \\ 91.9 + 3$		20 1 19 8 - 19 3 17 7	95 202.905	$0.38 \times 10^{-8}$	556 4
$\begin{array}{c} 32 2 4 7 - 4 1 3 6 \\ 32 2 0 - 32 3 29 0 \\ 34 4 31 1 - 35 2 34 1 \\ 103 354.03 78.41 \\ 1.03 \times 10^{-8} \\ 1.03 \times 10^{-8} \\ 587.9 \\ 32 2 30 5 - 33 0 33 5 \\ 103 395.991 \\ 3.64 \times 10^{-9} \\ 711.1 \\ 36 5 32 1 - 373 35 1 \\ 103 420.039 \\ 1.42 \times 10^{-8} \\ 674.0 \\ 11 2 9 3 - 11 1 10 3 \\ 103 456.903 \\ 4.86 \times 10^{-6} \\ 275.9 \\ 30 8 23 3 - 31 7 24 3 \\ 103 496.63 44 \\ 9.90 \times 10^{-7} \\ 779.4 \\ 30 8 22 3 - 31 7 25 3 \\ 103 496.544 \\ 9.90 \times 10^{-7} \\ 779.4 \\ 794.4 \\ 9.90 \times 10^{-7} \\ 794.4 \\ 10^{-7} \\ 755.2 \\ 22 3 20 - 3 - 23 0 23 - 3 \\ 90 903.575 \\ 2.41 \times 10^{-7} \\ 655.2 \\ 22 3 20 - 3 - 23 0 23 - 3 \\ 90 904.355 \\ 2.60 \times 10^{-8} \\ 452.6 \\ 51 50 - 41 4 0 \\ 90 905.1.8 \\ 2.44 \times 10^{-5} \\ 154. \\ 51 5 - 41 4 4 \\ 90 9051.18 \\ 2.44 \times 10^{-5} \\ 154. \\ 29 2 27 - 2 - 28 4 24 - 2 \\ 91 172.915 \\ 1.78 \times 10^{-8} \\ 766.8 \\ 29 2 27 - 2 - 28 4 24 - 2 \\ 91 172.915 \\ 1.78 \times 10^{-8} \\ 766.8 \\ 29 2 27 - 2 - 28 4 24 - 2 \\ 91 172.915 \\ 1.78 \times 10^{-8} \\ 767.6 \\ 52 2 \\ 23 1 22 1 - 22 3 19 1 \\ 91 305.92 \\ 1.01 \times 10^{-7} \\ 722.2 \\ 23 2 2 10 - 3 - 12 1 1 10 - 2 \\ 91 386.732 \\ 7.84 \times 10^{-7} \\ 722.2 \\ 39 5 35 - 40 3 38 0 \\ 91 395.29 \\ 1.01 \times 10^{-7} \\ 722.2 \\ 39 5 35 - 40 3 38 0 \\ 91 395.29 \\ 1.01 \times 10^{-7} \\ 727.2 \\ 39 5 35 - 40 3 38 0 \\ 91 395.29 \\ 1.01 \times 10^{-7} \\ 727.2 \\ 39 5 35 - 40 3 38 0 \\ 91 395.29 \\ 1.01 \times 10^{-7} \\ 815.7 \\ 50 5 1 - 4 0 4 1 \\ 93 192.298 \\ 2.70 \times 10^{-5} \\ 1.48 \\ 16 3 13 5 - 15 4 12 4 \\ 90 703.424 \\ 2.39 \times 10^{-5} \\ 1.48 \\ 16 3 13 5 - 15 4 12 4 \\ 90 703.424 \\ 2.39 \times 10^{-5} \\ 1.48 \\ 16 3 13$		554501-542551 5247 4128	103 321.08/	$1.00 \times 10^{-9}$	330.4 401.5
$\begin{array}{c} 332  232  0  323  234  0 \\ 344  311  -352  324  1 \\ 322  305  -330  335 \\ 322  305  -330  335 \\ 322  305  -330  335 \\ 322  305  -337  335  1 \\ 333  355  991 \\ 3.64  \times 10^{-9} \\ 711.1 \\ 365  321  -373  351 \\ 303  829  039  1.42  \times 10^{-8} \\ 674.0 \\ 308  223  -317  223 \\ 308  223  -317  223 \\ 308  223  -317  223 \\ 308  223  -317  223 \\ 308  223  -317  223 \\ 308  223  -317  225 \\ 308  223  -328  622  -3 \\ 907  907  905  909  \times 10^{-7} \\ 7794 \\ 7704 \\ 7707 \\ 7794 \\ 7704 \\ 7707 \\ 7794 \\ 7707 \\ 7794 \\ 7707 \\ 7704 \\ 7707 \\ 7704 \\ 7707 \\ 7704 \\ 7707 \\ 7704 \\ 7707 \\ 7704 \\ 7707 \\ 7704 \\ 7707 \\ 7704 \\ 7707 \\ 7704 \\ 7707 \\ 7707 \\ 7704 \\ 7707 \\ 7704 \\ 7707 \\ 7707 \\ 7704 \\ 7707 \\ 7704 \\ 7707 \\ 7704 \\ 7707 \\ 7707 \\ 7704 \\ 7707 \\ 7707 \\ 7704 \\ 7707 \\ 7707 \\ 7704 \\ 7707 \\ 7707 \\ 7707 \\ 7704 \\ 7707 \\ 7704 \\ 7707 \\ 7704 \\ 7707 \\ 7704 \\ 7707 \\ 7707 \\ 7704 \\ 7707 \\ 7707 \\ 7707 \\ 7704 \\ 7707 \\ 770$		5247-4138	103 326.134	$2.76 \times 10^{-7}$	401.5
$\begin{array}{c} 34 + 31 1 = 32 2 34 1 \\ 32 2 30 5 - 33 0 33 5 \\ 32 2 30 5 - 33 0 35 5 \\ 36 3 2 1 - 37 3 35 1 \\ 103 349,039 \\ 1.42 \times 10^{-8} 674,0 \\ 11 2 9 3 - 11 1 10 3 \\ 30 429,039 \\ 1.42 \times 10^{-8} 674,0 \\ 11 2 9 3 - 11 1 10 3 \\ 30 429,039 \\ 1.42 \times 10^{-8} 674,0 \\ 11 2 9 3 - 31 7 24 3 \\ 30 482 23 - 31 7 24 3 \\ 30 482 23 - 31 7 24 3 \\ 30 496,344 \\ 9.90 \times 10^{-7} 779,4 \\ \hline \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \$		35 2 32 0 - 32 5 29 0	103 334.08/	$1.84 \times 10^{-8}$	520.8
$\begin{array}{c} 32 2 3 0 - 33 0 3 3 \\ 36 5 3 21 - 37 3 5 1 \\ 11 2 9 3 - 11 1 10 3 \\ 103 456.903 \\ 4.86 \times 10^{-6} \\ 275.9 \\ 30 8 22 3 - 31 7 24 3 \\ 103 489.605 \\ 9.90 \times 10^{-7} \\ 779.4 \\ 30 8 22 3 - 31 7 25 3 \\ 103 496.34 \\ 9.90 \times 10^{-7} \\ 779.4 \\ 1^{15} CH_3 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 \\ 22 3 20 - 3 - 23 0 23 - 3 \\ 90 904.355 \\ 2.60 \times 10^{-8} \\ 452.6 \\ 51 5 0 - 41 40 \\ 90 995.753 \\ 2.41 \times 10^{-5} \\ 15.4 \\ 51 5 1 - 41 41 \\ 90 9951.18 \\ 2.41 \times 10^{-5} \\ 15.4 \\ 51 5 1 - 41 4.1 \\ 90 9951.18 \\ 2.41 \times 10^{-5} \\ 15.4 \\ 51 5 - 3 - 41 4 - 3 \\ 91 052.078 \\ 2.44 \times 10^{-5} \\ 21.8 \\ 34 4 31 - 3 - 34 2 33 - 3 \\ 90 9061.839 \\ 1.73 \times 10^{-8} \\ 746.1 \\ 51 5 - 3 - 41 4 - 3 \\ 91 052.078 \\ 2.44 \times 10^{-5} \\ 21.8 \\ 34 4 31 - 3 - 52 4 2 4 - 2 \\ 91 172.915 \\ 1.78 \times 10^{-8} \\ 612.2 \\ 25 3 23 - 26 0 26 - 3 \\ 91 232.409 \\ 2.32 \times 10^{-8} \\ 51.5 \\ 41 - 42 21 \\ 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} \\ 75.6 \\ 51 - 40 41 \\ 93 192.298 \\ 2.70 \times 10^{-5} \\ 13.5 \\ 36 9 28 - 3 78 8 29 - 3 \\ 93 194.864 \\ 8.16 \times 10^{-7} \\ 985.7 \\ 50 5 1 - 40 41 \\ 93 192.298 \\ 2.70 \times 10^{-5} \\ 13.5 \\ 36 9 28 - 3 78 8 29 - 3 \\ 93 194.864 \\ 8.16 \times 10^{-7} \\ 985.7 \\ 50 5 1 - 40 41 \\ 93 192.298 \\ 2.70 \times 10^{-5} \\ 13.5 \\ 36 9 28 - 3 78 8 29 - 3 \\ 93 194.864 \\ 8.16 \times 10^{-7} \\ 985.7 \\ 50 5 1 - 4 1 4 1 \\ 90 703.205 \\ 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 \\ 51 5 3 - 41 4 3 \\ 90 773.736 \\ 2.41 \times 10^{-8} \\ 341.6 \\ 14 2 2 3 - 41 3 3 \\ 90 798.85 \\ 2.55 \times 10^{-6} \\ 235.5 \\ 82 6 0 - 81 7 0 \\ 90 918.912 \\ 3.66 \times 10^{-7} \\ 39.8 \\ 14 3 12 3 - 150 15 3 \\ 90 926.52 \\ 2.93 \times 10^{-8} \\ 311.4 \\ 17 2 16 1 - 16 3 13 2 \\ 90 947.817 \\ 4.54 \times 10^{-7} \\ 14.3 \\ 11 5 6 2 - 12 4 8 \\ 91 192.805 \\ 5.21 \times 10^{-7} \\ 14.3 \\ 11 5 6 2 - 12 4 8 \\ 91 192.805 \\ 5.21 \times 10^{-7} \\ 315.3 \\ 22 8 14 5 - 23 7 16 \\ 91 278.76 \\ 6.004 \times 10^{-7} \\ 39.8 \\ 16 116 1 - 15$		34 4 31 1 - 33 2 34 1	103 378.41	$1.05 \times 10^{-9}$	J87.9 711.1
$ \begin{array}{c} 360 3 32 1 - 37 3 33 1 \\ 11 2 3 3 - 11 1 0 3 \\ 310 3 429 3 - 31 1 1 0 3 \\ 308 22 3 - 31 7 24 3 \\ 308 22 3 - 31 7 24 3 \\ 308 22 3 - 31 7 25 3 \\ 103 496 344 9.90 \times 10^{-7} 779.4 \\ 308 22 3 - 31 7 25 3 \\ 103 496 344 9.90 \times 10^{-7} 779.4 \\ 308 22 3 - 31 7 25 3 \\ 103 496 344 9.90 \times 10^{-7} 79.4 \\ 312 1 - 32 8 6 22 - 3 \\ 90 76 5.09 7 \\ 7.94 \times 10^{-7} 655.2 \\ 22 3 0 - 3 - 28 6 23 - 3 \\ 90 80 0.2 \\ 6.92 \times 10^{-8} 132.8 \\ 27 7 2 0 - 3 - 28 6 23 - 3 \\ 90 90 90 1.095 \\ 7.33 \times 10^{-7} 655.2 \\ 22 3 0 - 3 - 23 0 23 - 3 \\ 90 990 1.355 \\ 2.60 \times 10^{-8} 452.6 \\ 51 5 0 - 41 4 0 \\ 90 995 5.753 \\ 2.41 \times 10^{-5} 15.4 \\ 51 5 1 - 41 4 1 \\ 90 995 1.18 \\ 2.41 \times 10^{-5} 15.4 \\ 51 5 1 - 41 4 - 3 \\ 91 052 078 \\ 2.44 \times 10^{-5} 15.4 \\ 51 5 3 - 41 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} 61.2 \\ 25 3 23 - 3 - 20 23 27 - 3 \\ 91 304.282 \\ 6.05 \times 10^{-7} 620.5 \\ 52 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} 985.7 \\ 39 4 36 - 3 - 40 2 39 - 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 \\ 103 453.152 \\ 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} 837.5 \\ 39 4 36 - 3 - 40 2 39 - 3 \\ 103 353.904 \\ 2.05 \times 10^{-5} 14.8 \\ 51 5 1 - 4 1 4 1 \\ 90 703.424 \\ 2.39 \times 10^{-5} 14.8 \\ 51 5 1 - 4 1 4 1 \\ 90 707.3424 \\ 2.39 \times 10^{-5} 14.8 \\ 51 5 1 - 4 1 4 1 \\ 90 707.3424 \\ 2.39 \times 10^{-5} 14.8 \\ 51 5 1 - 4 1 4 1 \\ 90 707.3424 \\ 2.39 \times 10^{-5} 14.8 \\ 51 5 1 - 4 1 4 1 \\ 90 707.3424 \\ 2.39 \times 10^{-5} 14.8 \\ 51 5 1 - 4 1 4 1 2 4 \\ 90 707.948 \\ 5.88 \times 10^{-8} 341.0 \\ 51 5 3 - 4 1 4 3 90 779.352 \\ 2.29 \times 10^{-5} 14.5 \\ 14 - 2 1 3 18 2 \\ 90 947.817 \\ 4.58 \times 10^{-7} 144.3 \\ 11 5 6 2 - 1$		32 2 30 3 - 33 0 33 3 26 5 20 1 - 27 2 25 1	103 393.991	$3.04 \times 10^{-8}$	/11.1
$ \begin{array}{c} 112 9 3 - 111 10 3 \\ 30 8 23 3 - 31 7 24 3 \\ 30 8 22 3 - 31 7 25 3 \\ 103 496.344 \\ 9.00 \times 10^{-7} \\ 779.4 \\ 1^3 CH_3 CHO \\ 27 7 21 - 3 - 28 6 22 - 3 \\ 27 7 21 - 3 - 28 6 22 - 3 \\ 27 7 20 - 3 - 28 6 23 - 3 \\ 22 3 20 - 3 - 23 0 23 - 3 \\ 90 904.355 \\ 22 0 20 - 3 - 23 0 23 - 3 \\ 90 904.355 \\ 2.60 \times 10^{-8} \\ 132.8 \\ 27 7 20 - 3 - 28 6 23 - 3 \\ 90 904.355 \\ 2.60 \times 10^{-8} \\ 155 \\ 22 3 20 - 3 - 23 0 23 - 3 \\ 90 904.355 \\ 2.60 \times 10^{-8} \\ 151 \\ 51 5 0 - 41 4 0 \\ 90 9951.18 \\ 2.41 \times 10^{-5} \\ 154 \\ 51 5 1 - 41 41 \\ 90 9051.18 \\ 2.41 \times 10^{-5} \\ 154 \\ 33 4 3 0 - 3 42 23 - 3 \\ 91 0052.078 \\ 2.44 \times 10^{-5} \\ 221.8 \\ 34 4 31 - 3 - 35 2 34 - 3 \\ 91 052.078 \\ 2.44 \times 10^{-5} \\ 221.8 \\ 34 4 31 - 3 - 35 2 34 - 3 \\ 91 052.078 \\ 2.44 \times 10^{-5} \\ 221.8 \\ 34 4 31 - 3 - 35 2 34 - 3 \\ 91 052.078 \\ 2.44 \times 10^{-5} \\ 221.8 \\ 34 4 31 - 3 - 35 2 34 - 3 \\ 91 052.078 \\ 2.44 \times 10^{-5} \\ 221.8 \\ 34 4 31 - 3 - 35 2 34 - 3 \\ 91 052.078 \\ 2.44 \times 10^{-5} \\ 221.8 \\ 326 - 3 - 29 3 27 - 3 \\ 91 304.282 \\ 6.05 \times 10^{-7} \\ 620.5 \\ 52 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 \\ 8.31 \times 10^{-7} \\ 511.6 \\ 112 10 - 2 - 111 10 - 2 \\ 91 386.732 \\ 7.84 \times 10^{-7} \\ 772.2 \\ 39 5 35 0 - 40 3 38 0 \\ 91 395.629 \\ 8.97 \times 10^{-9} \\ 758.9 \\ 36 9 27 - 3 - 37 8 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} \\ 318.3 \\ 16 3 - 10 0 19 - 3 \\ 103 463.152 \\ 4.01 \times 10^{-8} \\ 378.7 \\ 12 2 10 - 3 - 12 1 11 - 3 \\ 103 487.851 \\ 5.26 \times 10^{-6} \\ 285.2 \\ CH_3 CDO \\ 51 5 0 - 41 4 0 \\ 90 707.342 \\ 2.39 \times 10^{-5} \\ 14.8 \\ 51 5 3 - 41 4 3 \\ 90 773.736 \\ 2.41 \times 10^{-8} \\ 314. \\ 16 3 13 5 - 15 4 12 4 \\ 90 707.948 \\ 5.88 \times 10^{-8} \\ 341.0 \\ 51 5 3 - 41 4 3 \\ 90 773.736 \\ 2.41 \times 10^{-7} \\ 232.9 \\ 10 1 9 5 - 10 0 10 5 \\ 90 849.045 \\ 2.77 \times 10^{-6} \\ 235.2 \\ CH_3 CDO \\ 51 5 1 - 41 4 1 \\ 10 2 90 973.81 \\ 2.05 \times 10^{-7} \\ 14.3 \\ 11 5 6 2 - 12 4 8 2 \\ 91 192.805 \\ 5.21 \times 10^{-7} \\ 14.3 \\ 11 5 6 2 - 12 4 8 2 \\ 91 192.805 \\ 5.21 \times 10^{-7} \\ 14.3 \\ 11 5 6 2 - 12 4 8 \\ 21 10 3 300.073 \\ 9.11 \times$		30 3 32 1 - 37 3 33 1 11 2 0 2 11 1 1 0 2	103 429.039	$1.42 \times 10^{-6}$	074.0
$\begin{array}{c} 308\ 223 - 31\ 724\ 3 \\ 30\ 8\ 223 - 31\ 7\ 25\ 3 \\ 103\ 496\ 344\ 9.90\ \times10^{-7}\ 779.4 \\ 1^{15}\mbox{CH}_3\mbox{CH}_3\ CH_3\ CH_3$		11 2 9 3 - 11 1 10 3	103 430.905	$4.80 \times 10^{-7}$	273.9
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		30 8 23 3 - 31 7 24 3	103 489.003	$9.90 \times 10^{-7}$	779.4
$\begin{array}{c} 37632-3-36729-3 \\ 27721-3-28622-3 \\ 162141-153121 \\ 90802.2 \\ 6.92\times10^{-8} \\ 1328 \\ 27720-3-28623-3 \\ 90904.355 \\ 2.60\times10^{-8} \\ 1328 \\ 27720-3-28623-3 \\ 90904.355 \\ 2.60\times10^{-8} \\ 452.6 \\ 5150-4140 \\ 90935753 \\ 2.41\times10^{-5} \\ 15.4 \\ 33430-3-34233-3 \\ 90961.839 \\ 1.73\times10^{-8} \\ 746.1 \\ 5153-414-3 \\ 91052.078 \\ 2.41\times10^{-5} \\ 15.4 \\ 33430-3-34233-3 \\ 90961.839 \\ 1.73\times10^{-8} \\ 746.1 \\ 5153-414-3 \\ 91058.163 \\ 1.68\times10^{-8} \\ 776.8 \\ 29227-2-28424-2 \\ 91172.915 \\ 1.78\times10^{-8} \\ 612.2 \\ 25323-3-26026-3 \\ 91232.409 \\ 2.32\times10^{-8} \\ 517.4 \\ 29326-3-29327-3 \\ 91305.92 \\ 1.01\times10^{-7} \\ 22.5 \\ 231221-223191 \\ 91313.98 \\ 3.30\times10^{-8} \\ 253.5 \\ 325280-316250 \\ 91370.438 \\ 8.31\times10^{-7} \\ 515.6 \\ 11210-2-11110-2 \\ 91386.732 \\ 7.84\times10^{-7} \\ 985.7 \\ 5051-4041 \\ 93192.298 \\ 2.70\times10^{-5} \\ 1.6\times10^{-7} \\ 985.7 \\ 39436-3-40239-3 \\ 103353.904 \\ 2.05\times10^{-8} \\ 943.5 \\ 18316-3-19019-3 \\ 103463.152 \\ 4.01\times10^{-8} \\ 378.7 \\ 38534-2.39237-2 \\ 103484.196 \\ 7.87\times10^{-8} \\ 943.5 \\ 18316-3-19019-3 \\ 103463.152 \\ 4.01\times10^{-8} \\ 378.7 \\ 38534-2.39237-2 \\ 103484.196 \\ 7.87\times10^{-8} \\ 943.5 \\ 18316-3-19019-3 \\ 103463.152 \\ 4.01\times10^{-8} \\ 378.7 \\ 39436-3-40239-3 \\ 103353.904 \\ 2.05\times10^{-8} \\ 943.5 \\ 14.8 \\ 163135-154124 \\ 90707.326 \\ 2.39\times10^{-5} \\ 14.8 \\ 163135-154124 \\ 90707.342 \\ 2.39\times10^{-5} \\ 14.8 \\ 163135-154124 \\ 90773.736 \\ 2.41\times10^{-5} \\ 216.4 \\ 4223-4133 \\ 90779.825 \\ 2.55\times10^{-6} \\ 217.0 \\ 222211-213182 \\ 90823.11 \\ 2.02\times10^{-7} \\ 232.9 \\ 10195-100105 \\ 90849.045 \\ 2.77\times10^{-6} \\ 25.5 \\ 82.60-8170 \\ 90918.912 \\ 3.66\times10^{-6} \\ 39.8 \\ 143123-150153 \\ 90926.592 \\ 2.93\times10^{-5} \\ 14.8 \\ 1562-12482 \\ 91192.805 \\ 5.21\times10^{-7} \\ 315.3 \\ 28145-237165 \\ 91278.766 \\ 6.04\times10^{-7} \\ 539.8 \\ 161161-153134 \\ 10330.0737 \\ 911\times10^{-7} \\ 539.8 \\ 161161-153134 \\ 10330.0737 \\ 911\times10^{-7} \\ 539.8 \\ 161161-153134 \\ 10330.073 \\ 911\times10^{-7} \\ 329.6 \\ 2014-2124 \\ 103470.435 \\ 2244\times19\times10^{-6} \\ 209.1 \\ 214-2124 \\ 103470.435 \\ 2244\times19\times10^{-6} \\ 209.1 \\ 2014-2124 \\ 103470.435 \\ 2244\times105 \\ 310-6^{-6} \\ 39.8 \\ 310-7^{-7} \\ 315.3 \\ 315.5215124-2246194 \\ 103$		30 8 22 3 - 31 7 25 3	103 490.344	$9.90 \times 10^{-7}$	//9.4
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	"CH <sub>3</sub> CHO	37 0 32 -3 - 30 7 29 -3	90 703.097	$7.94 \times 10^{-7}$	918.8
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		27 7 21 -3 - 28 0 22 -3	90 /91.095	$7.33 \times 10^{-8}$	122.9
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		16 2 14 1 - 15 3 12 1	90 802.2	$6.92 \times 10^{-7}$	132.8
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		27 7 20 -3 - 28 6 23 -3	90 830.059	$7.34 \times 10^{-8}$	055.2 452.6
$\begin{array}{c} 5130-4140 \\ 5151-4141 \\ 90951.18 \\ 2.41\times10^{-5} \\ 154 \\ 33430-3-34233-3 \\ 90961.839 \\ 1.73\times10^{-8} \\ 746.1 \\ 515-3-414-3 \\ 91052.078 \\ 2.44\times10^{-5} \\ 221.8 \\ 34431-3-35234-3 \\ 91058.163 \\ 1.68\times10^{-8} \\ 776.8 \\ 29227-2-28424-2 \\ 91172.915 \\ 1.78\times10^{-8} \\ 612.2 \\ 25323-3-26026-3 \\ 91232.409 \\ 2.32\times10^{-8} \\ 517.4 \\ 29326-3-29327-3 \\ 91304.282 \\ 6.05\times10^{-7} \\ 620.5 \\ 5241-4221 \\ 91305.92 \\ 1.01\times10^{-7} \\ 22.5 \\ 231221-223191 \\ 91313.98 \\ 3.30\times10^{-8} \\ 253.5 \\ 325280-316250 \\ 91370.438 \\ 8.31\times10^{-7} \\ 515. \\ 325280-316250 \\ 91370.438 \\ 8.31\times10^{-7} \\ 727.2 \\ 395350-403380 \\ 91395.629 \\ 8.97\times10^{-9} \\ 758.9 \\ 36928-3-37829-3 \\ 93187.027 \\ 8.16\times10^{-7} \\ 985.7 \\ 39436-3-40239-3 \\ 103353.904 \\ 2.05\times10^{-8} \\ 943.5 \\ 18316-3-19019-3 \\ 103463.152 \\ 4.01\times10^{-8} \\ 378.7 \\ 38534-2-39237-2 \\ 103484.196 \\ 7.87\times10^{-8} \\ 928.7 \\ 12210-3-12111-3 \\ 103487.851 \\ 5.26\times10^{-6} \\ 285.2 \\ CH_{3}CDO \\ 5150-4140 \\ 90703.205 \\ 2.39\times10^{-5} \\ 14.8 \\ 5151-4.4141 \\ 90707.948 \\ 5.88\times10^{-8} \\ 341.0 \\ 5155-4.2143 \\ 90779.825 \\ 2.55\times10^{-6} \\ 217.0 \\ 222211-213182 \\ 90823.11 \\ 2.02\times10^{-7} \\ 20241-213812 \\ 90823.11 \\ 2.02\times10^{-7} \\ 20241-213812 \\ 90849.045 \\ 2.77\times10^{-6} \\ 235.5 \\ 8260-8170 \\ 90918.912 \\ 3.66\times10^{-6} \\ 39.8 \\ 143123-150153 \\ 90926.592 \\ 2.93\times10^{-8} \\ 311.4 \\ 172161-163132 \\ 90947.817 \\ 4.54\times10^{-7} \\ 315.3 \\ 228145-237165 \\ 91278.766 \\ 6.04\times10^{-7} \\ 39.7 \\ 2512132-246194 \\ 103300.073 \\ 9.11\times10^{-7} \\ 315.3 \\ 228145-237165 \\ 91278.766 \\ 6.04\times10^{-7} \\ 39.7 \\ 2512132-246194 \\ 103300.073 \\ 9.11\times10^{-7} \\ 329.6 \\ 2214-2124 \\ 103470.435 \\ 2.49\times10^{-7} \\ 329.6 \\ 2.214-2124 \\ 103470.435 \\ 2.49\times10^{-7} \\ 329.6 \\ 2.214-2124 \\ 103470.435 \\ 2.49\times10^{-7} \\ 329.6 \\ 2.214-2124 \\ 103470.435 \\ 2.49\times10^{-7} \\ 329.6 \\ 2.249\times10^{-7} \\ 329.6 \\ 329.6 \\ 329.6 \\ 329.6 \\ 329.6 \\ 329.6 \\ 329.6 \\ 329$		22 5 20 -5 - 25 0 25 -5	90 904.555	$2.00 \times 10^{-5}$	432.0
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		5150 - 4140	90 955.755	$2.41 \times 10^{-5}$	15.4
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		5151-4141	90 951.18	$2.41 \times 10^{-8}$	15.4
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		33 4 30 -3 - 34 2 33 -3 5 1 5 2 4 1 4 2	90 901.839	$1.73 \times 10^{-5}$	/40.1
$\begin{array}{c} 34431-3-53234+3\\ 29227-2-28424-2\\ 91172.915\\ 1.78\times 10^{-8}\\ 612.2\\ 25323-3-26026-3\\ 91232.409\\ 2.32\times 10^{-8}\\ 517.4\\ 29326-3-29327-3\\ 91304.282\\ 6.05\times 10^{-7}\\ 620.5\\ 5241-4221\\ 91305.92\\ 1.01\times 10^{-7}\\ 22.5\\ 231221-223191\\ 91313.98\\ 3.30\times 10^{-8}\\ 253.5\\ 325280-316250\\ 91370.438\\ 8.31\times 10^{-7}\\ 531.6\\ 11210-2-11110-2\\ 91386.732\\ 74\times 10^{-7}\\ 758.9\\ 36927-3-37829-3\\ 93187.027\\ 8.16\times 10^{-7}\\ 985.7\\ 5051-4041\\ 93192.298\\ 2.70\times 10^{-5}\\ 13.5\\ 36928-3-37830-3\\ 93194.864\\ 8.16\times 10^{-7}\\ 985.7\\ 39436-3-40239-3\\ 103353.904\\ 2.05\times 10^{-8}\\ 943.5\\ 18316-3-19019-3\\ 103463.152\\ 4.01\times 10^{-8}\\ 928.7\\ 12210-3-12111-3\\ 103487.851\\ 5.26\times 10^{-6}\\ 285.2\\ \hline CH_3CDO\\ 5150-4140\\ 90773.265\\ 2.25\times 10^{-6}\\ 217.0\\ 222211-213182\\ 90779.825\\ 2.55\times 10^{-6}\\ 217.0\\ 222211-213182\\ 90823.11\\ 2.02\times 10^{-7}\\ 232.9\\ 10195-100105\\ 90849.045\\ 2.77\times 10^{-6}\\ 253.5\\ 8260-8170\\ 90918.912\\ 3.66\times 10^{-6}\\ 39.8\\ 143123-150153\\ 90926.592\\ 2.93\times 10^{-5}\\ 311.4\\ 172161-163132\\ 90947.817\\ 4.54\times 10^{-7}\\ 144.3\\ 11562-12482\\ 91192.805\\ 5.21\times 10^{-7}\\ 102.6\\ 152144-143124\\ 91214.539\\ 3.12\times 10^{-7}\\ 315.3\\ 228145-237165\\ 91278.766\\ 6.04\times 10^{-7}\\ 329.6\\ 2214-2124\\ 103300.073\\ 9.11\times 10^{-7}\\ 329.6\\ 2214-2124\\ 103470.435\\ 2.49\times 10^{-6}\\ 209.1\\ \hline$		5 1 5 - 5 - 4 1 4 - 5	91 052.078	$2.44 \times 10^{-8}$	221.8
$\begin{array}{c} 29227-2-28424-2 \\ 25323-3-26026-3 \\ 91232409 \\ 2.32\times10^{-8} \\ 517.4 \\ 29326-3-29327-3 \\ 91304.282 \\ 6.05\times10^{-7} \\ 620.5 \\ 5241-4221 \\ 91305.92 \\ 1.01\times10^{-7} \\ 22.5 \\ 231221-223191 \\ 91313.98 \\ 3.30\times10^{-8} \\ 253.5 \\ 325280-316250 \\ 91370.438 \\ 8.31\times10^{-7} \\ 51.6 \\ 11210-2-11110-2 \\ 91386.732 \\ 7.84\times10^{-7} \\ 727.2 \\ 395350-403380 \\ 91395.629 \\ 8.97\times10^{-9} \\ 758.9 \\ 36927-3-37829-3 \\ 93187.027 \\ 8.16\times10^{-7} \\ 985.7 \\ 5051-4041 \\ 93192.298 \\ 2.70\times10^{-5} \\ 13.5 \\ 36928-3-37830-3 \\ 93194.864 \\ 8.16\times10^{-7} \\ 985.7 \\ 39436-3-40239-3 \\ 103353.904 \\ 2.05\times10^{-8} \\ 943.5 \\ 18316-3-19019-3 \\ 103463.152 \\ 4.01\times10^{-8} \\ 928.7 \\ 12210-3-12111-3 \\ 103487.851 \\ 5.26\times10^{-6} \\ 285.2 \\ \hline CH_3CDO \\ 5150-4140 \\ 90703.205 \\ 2.39\times10^{-5} \\ 14.8 \\ 5151-4144 \\ 90779.424 \\ 2.39\times10^{-5} \\ 14.8 \\ 5151-4143 \\ 90777.376 \\ 2.41\times10^{-5} \\ 216.4 \\ 4223-4133 \\ 90799.825 \\ 2.55\times10^{-6} \\ 217.0 \\ 222211-213182 \\ 90823.11 \\ 2.02\times10^{-7} \\ 232.9 \\ 10195-100105 \\ 90849.045 \\ 2.77\times10^{-6} \\ 253.5 \\ 8260-8170 \\ 90918.912 \\ 3.66\times10^{-6} \\ 39.8 \\ 143123-150153 \\ 90926.592 \\ 2.93\times10^{-8} \\ 311.4 \\ 172161-163132 \\ 90947.817 \\ 4.54\times10^{-7} \\ 144.3 \\ 11562-12482 \\ 91192.805 \\ 5.21\times10^{-7} \\ 102.6 \\ 152144-143124 \\ 91214.539 \\ 3.12\times10^{-7} \\ 315.3 \\ 228145-237165 \\ 91278.766 \\ 6.04\times10^{-7} \\ 329.6 \\ 2214-2124 \\ 103300.073 \\ 9.11\times10^{-7} \\ 329.6 \\ 2214-2124 \\ 103470.435 \\ 2.49\times10^{-6} \\ 209.1 \\ 103470.435 \\$		34 4 31 -3 - 33 2 34 -3	91 038.105	$1.08 \times 10^{-8}$	//0.8
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		29 2 27 -2 - 28 4 24 -2	91 172.913	$1.78 \times 10^{-8}$	012.2 517.4
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		25 5 25 -5 - 20 0 20 -5	91 252.409	$2.32 \times 10^{-7}$	517.4 620.5
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		29 5 20 - 5 - 29 5 27 - 5	91 304.282	$0.03 \times 10^{-7}$	020.5
$\begin{array}{c c c c c c c c c c c c c c c c c c c $		3 2 4 1 - 4 2 2 1 22 1 22 1 22 2 10 1	91 303.92	$1.01 \times 10^{-8}$	22.3
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		25 1 22 1 - 22 5 19 1	91 313.96	$3.30 \times 10^{-7}$	233.3 521.6
$\begin{array}{c c c c c c c c c c c c c c c c c c c $		$32 \ 528 \ 0 - 51 \ 0 \ 25 \ 0$	91 370.430	$6.31 \times 10^{-7}$	222.2
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		20 5 25 0 40 2 28 0	91 300.732	$7.64 \times 10^{-9}$	758.0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		39 5 55 0 - 40 5 58 0	91 393.029	$8.97 \times 10^{-7}$	085 7
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		50514041	93 107.027	$3.10 \times 10^{-5}$	12.5
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		360.28 3 37.8 30 3	93 192.298	$2.70 \times 10^{-7}$	085.7
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		30 / 36 3 / 0 2 30 3	103 353 004	$3.10 \times 10^{-8}$	905.7
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		18 3 16 3 10 0 10 3	103 463 152	$2.03 \times 10^{-8}$	3787
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		38 5 34 _2 _ 39 2 37 _2	103 484 196	$7.87 \times 10^{-8}$	978.7
$\begin{array}{c c c c c c c c c c c c c c c c c c c $		$12 \ 2 \ 10 \ -3 \ -12 \ 11 \ 11 \ -3$	103 487 851	$5.26 \times 10^{-6}$	285.2
$\begin{array}{c} 5.13 \times 10^{-4} \times 14^{-0} & 5.0703.424 & 2.39 \times 10^{-5} & 14.8 \\ 5.151 - 4141 & 90703.424 & 2.39 \times 10^{-5} & 14.8 \\ 163135 - 154124 & 90707.948 & 5.88 \times 10^{-8} & 341.0 \\ 5153 - 4143 & 90773.736 & 2.41 \times 10^{-5} & 216.4 \\ 4223 - 4133 & 90799.825 & 2.55 \times 10^{-6} & 217.0 \\ 222211 - 213182 & 90823.11 & 2.02 \times 10^{-7} & 232.9 \\ 10195 - 100105 & 90849.045 & 2.77 \times 10^{-6} & 253.5 \\ 8260 - 8170 & 90918.912 & 3.66 \times 10^{-6} & 39.8 \\ 143123 - 150153 & 90926.592 & 2.93 \times 10^{-8} & 311.4 \\ 172161 - 163132 & 90947.817 & 4.54 \times 10^{-7} & 144.3 \\ 11562 - 12482 & 91192.805 & 5.21 \times 10^{-7} & 102.6 \\ 152144 - 143124 & 91214.539 & 3.12 \times 10^{-7} & 315.3 \\ 228145 - 237165 & 91278.766 & 6.04 \times 10^{-7} & 539.7 \\ 2512132 - 246194 & 103300.073 & 9.11 \times 10^{-7} & 539.8 \\ 161161 - 153134 & 103316.694 & 3.40 \times 10^{-7} & 329.6 \\ 2214 - 2124 & 103470.435 & 2.49 \times 10^{-6} & 209.1 \end{array}$	CH_CDO	5150-4140	90 703 205	$\frac{3.20 \times 10}{2.39 \times 10^{-5}}$	14.8
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	CH3CDO	5150 - 4140 5151 - 4141	90 703 424	$2.37 \times 10^{-5}$	14.8
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		163135-154124	90 707 948	$5.88 \times 10^{-8}$	341.0
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		5153-4143	90773736	$2.00 \times 10^{-5}$	216.4
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		4223-4133	90 799 825	$2.41 \times 10^{-6}$ 2.55 × 10 <sup>-6</sup>	210.4
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		22 2 21 1 - 21 3 18 2	90 823 11	$2.03 \times 10^{-7}$ 2.02 × 10 <sup>-7</sup>	232.9
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		10195 - 100105	90 849 045	$2.02 \times 10^{-6}$ 2.77 × 10 <sup>-6</sup>	253.5
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		8260-8170	90 918 912	$3.66 \times 10^{-6}$	39.8
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		14 3 12 3 - 15 0 15 3	90 926 592	$2.93 \times 10^{-8}$	311.4
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		17 2 16 1 - 16 3 13 2	90 947 817	$4.54 \times 10^{-7}$	144.3
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		11562-12482	91 192 805	$5.21 \times 10^{-7}$	102.6
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		15 2 14 4 - 14 3 12 4	91 214 539	$3.12 \times 10^{-7}$	315.3
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		22.8.14.5 - 23.7.16.5	91 278 766	$6.04 \times 10^{-7}$	5397
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		25 12 13 2 - 24 6 19 4	103 300 073	$9.11 \times 10^{-7}$	539.8
$\begin{array}{c} 101101 & 105101 \\ 2214 - 2124 \\ 103470.435 & 2.49 \times 10^{-6} \\ 209.1 \end{array}$		16 11 6 1 - 15 3 13 4	103 316 694	$3.40 \times 10^{-7}$	329.6
		2214-2124	103 470.435	$2.49 \times 10^{-6}$	209.1

$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$	~ .				
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	Species	Transition	Frequency	$A_{ij}$	$E_{up}$
$\begin{array}{c} {\rm CH}_{3}{\rm DCHO} & 6 \ 3 \ 4 \ 2 \ - \ 7 \ 2 \ 6 \ 1 \\ & 5 \ 2 \ 3 \ 1 \ + \ 2 \ 3 \ 2 \\ & 5 \ 2 \ 3 \ 1 \ + \ 2 \ 3 \ 2 \\ & 5 \ 2 \ 3 \ 2 \ + \ 2 \ 3 \ 1 \\ & 5 \ 2 \ 3 \ 2 \ + \ 2 \ 4 \ 2 \ 3 \ 1 \\ & 5 \ 2 \ 3 \ 2 \ - \ 4 \ 2 \ 1 \\ & 5 \ 2 \ 3 \ 2 \ - \ 4 \ 2 \ 1 \\ & 5 \ 2 \ 3 \ 2 \ - \ 4 \ 3 \ 1 \ 3 \ 1 \ 3 \ 0 \ - \ 7 \ 4 \ 3 \ 7 \\ & 5 \ 2 \ 3 \ 2 \ - \ 4 \ 2 \ 1 \ 1 \ 1 \ 2 \ - \ 1 \ 3 \ 1 \ 3 \ 1 \ 2 \ - \ 1 \ 3 \ 1 \ 3 \ 1 \ 3 \ 2 \ 1 \ 1 \ 1 \ 1 \ 1 \ 1 \ 1 \ 1 \ 1$		JKLM	(MHz)	$(s^{-1})$	(K)
$ \begin{array}{c} 5 & 2 & 3 & 1 - 4 & 2 & 3 & 2 \\ 5 & 2 & 3 & 2 - 4 & 2 & 3 & 1 \\ 5 & 2 & 3 & 2 - 4 & 2 & 3 & 1 \\ 1 & 3 & 1 & 0 & - 2 & 0 & 2 & 0 \\ 1 & 3 & 1 & 1 & 2 & - 1 & 3 & 0 & 1 & 3 & 0 & 2 & 0 & - 1 & 6 & 7 & 0 \\ 1 & 3 & 1 & 1 & 2 & 1 & 3 & 0 & 1 & 3 & 0 & 2 & 1 & 0 & - 1 & 3 & 0 & 2 & 1 & 0 & - 1 & 1 & 0 & 1 & 1 \\ 1 & 1 & 2 & 0 & - 1 & 3 & 0 & 1 & 3 & 1 & 0 & 1 & 3 & 3 & 0 & 2 & 1 & 0 & - 1 & 6 & 1 & 0 & 4 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0$	CH <sub>2</sub> DCHO	6342-7261	90 671.76	$1.70 \times 10^{-7}$	59.2
$ \begin{array}{c} 5 2 3 2 - 4 2 3 1 \\ 3 1 3 0 - 2 0 2 0 \\ 1 3 1 1 2 2 - 13 0 13 2 \\ 1 3 1 1 2 2 - 13 0 13 2 \\ 1 1 0 - 13 1 1 2 1 - 13 0 13 1 \\ 1 1 2 1 - 13 0 13 1 \\ 1 1 2 1 - 13 0 13 1 \\ 1 1 2 1 - 13 0 13 1 \\ 1 1 2 1 - 13 0 13 1 \\ 1 1 2 1 - 13 0 13 1 \\ 1 1 3 1 4 - 7 2 6 2 \\ 1 1 3 1 4 - 7 2 6 2 \\ 1 1 3 1 4 - 7 2 6 2 \\ 1 1 3 1 4 - 7 2 6 2 \\ 1 1 3 1 2 - 1 3 0 1 3 \\ 1 1 1 1 1 1 0 - 5 \\ 1 0 3 3 0 8 . 4 3 1 \\ 1 - 1 1 1 1 0 - 5 \\ 1 0 3 4 0 3 8 1 \\ 1 - 1 1 1 1 0 - 5 \\ 1 0 3 4 0 3 8 1 \\ 1 - 1 1 1 1 0 - 5 \\ 1 0 3 4 0 3 8 1 \\ 1 - 1 1 1 1 0 - 5 \\ 1 0 3 4 0 3 8 1 \\ 1 - 1 1 1 1 0 - 5 \\ 1 0 3 4 0 3 8 3 \\ 1 - 5 1 - 5 1 \\ 1 0 3 4 0 3 8 3 \\ 1 - 5 1 - 5 1 \\ 1 0 3 4 0 3 8 3 \\ 1 - 5 1 - 5 1 \\ 1 0 3 4 0 3 1 \\ 1 - 5 1 5 1 \\ 1 0 3 4 0 3 1 \\ 1 - 5 1 5 1 \\ 1 0 3 4 0 5 1 \\ 1 0 3 4 0 3 1 \\ 1 - 7 \\ 1 - 6 0 6 - 5 0 5 0 \\ 1 0 3 4 8 0 - 7 \\ 1 - 7 \\ 1 - 6 0 6 - 5 0 5 0 \\ 1 0 3 4 8 0 - 7 \\ 1 - 7 \\ 1 - 6 0 6 - 5 0 5 0 \\ 1 0 3 4 8 0 - 7 \\ 1 - 7 \\ 1 - 6 0 6 - 5 0 5 0 \\ 1 0 3 4 8 0 - 7 \\ 1 - 7 \\ 1 - 7 \\ 1 - 6 0 6 - 5 0 5 0 \\ 1 0 3 4 8 0 - 7 \\ 1 - 7 \\ 1 - 7 \\ 1 - 7 \\ 1 - 6 0 6 - 5 0 5 0 \\ 1 0 3 4 8 0 - 7 \\ 1 -$		5231-4232	90 897.364	$4.40 \times 10^{-7}$	43.7
$ \begin{array}{c} 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^{-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 2 0 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 4450.4 & 1.69 \times 10^{-8} & 151.2 \\ 11 2 10 1 - 11 1 10 2 & 103 4450.4 & 1.69 \times 10^{-8} & 151.2 \\ 11 2 10 1 - 11 1 10 2 & 103 4473.67 & 3.75 \times 10^{-9} & 40.1 \\ 6 0 6 1 - 5 0 5 1 & 103 4473.67 & 3.75 \times 10^{-9} & 17.4 \\ 6 0 6 0 - 5 0 5 0 & 103 480.72 & 3.72 \times 10^{-9} & 17.4 \\ 6 0 6 0 - 5 0 5 0 & 103 480.72 & 3.72 \times 10^{-9} & 916.5 \\ 39 13 26 1 - 38 14 24 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 0 46 1 & 90 673.816 & 3.95 \times 10^{-8} & 916.6 \\ 47 2 46 2 - 46 1 46 1 & 90 673.816 & 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 \\ 47 2 46 2 - 46 0 46 1 & 90 674.571 & 1.70 \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} & 491.7 \\ 28 12 16 2 - 29 11 18 2 & 90 736.57 & 7.33 \times 10^{-7} & 521.5 \\ 28 12 16 2 - 29 11 18 2 & 90 736.57 & 7.33 \times 10^{-7} & 521.5 \\ 38 6 33 1 - 39 7 33 2 & 90 809.192 & 1.68 \times 10^{-8} & 694.1 \\ 21 2 0 2 2 - 21 19 3 0 & 90 947.962 & 6.04 \times 10^{-8} & 694.1 \\ 21 2 0 1 2 - 21 19 2 0 & 90 947.962 & 6.04 \times 10^{-8} & 694.1 \\ 21 2 0 1 2 - 21 19 2 0 & 90 947.962 & 6.04 \times 10^{-8} & 694.1 \\ 21 2 0 2 2 - 71 - 97 732 2 & 90 992.97 & 8.40 \times 10^{-8} & 433.1 \\ 14 2 13 2 - 13 3 10 2 & 91 007.73 & 99 1 \times 10^{-7} & 89.7 \\ 35 10 26 1 - 35 11 26 1 & 91 030.651 & 3.31 \times 10^{-8} & 73.8 \\ 36 10 26 1 - 35 11 25 1 & 91 030.6631 & 3.31 \times 10^{-8} & 73.8 \\ 36 10 26 1 - 35 11 25 1 & 91 030.6631 & 3.31 \times 10^{-8} & 73.8 $		5232-4231	90979.724	$2.97 \times 10^{-7}$	43.7
$ \begin{array}{c} 13 1 12 2 - 13 0 13 2 \\ 18 2 16 0 - 18 2 17 0 \\ 13 0 13 1 \\ 21 1 - 13 0 13 1 \\ 21 1 - 13 0 13 1 \\ 25 8 18 0 - 26 7 19 0 \\ 25 8 18 0 - 26 7 19 0 \\ 25 8 18 0 - 26 7 19 0 \\ 10 3 303 8.17 \\ 1.11 \times 10^{-6} \\ 409.4 \\ 25 8 17 0 - 26 7 20 0 \\ 10 3 303 8.17 \\ 1.11 \times 10^{-6} \\ 409.4 \\ 16 4 12 0 - 17 2 15 0 \\ 10 3 450.4 \\ 1.69 \times 10^{-8} \\ 87.7 \\ \hline \\ $		3 1 3 0 - 2 0 2 0	91 090.016	$3.43 \times 10^{-6}$	7.0
$ \begin{array}{c} 18\ 2\ 16\ 0\ -\ 18\ 2\ 17\ 0\ 9\ 1\ 308\ 321\ 5\ 09\ \times\ 10^{-7}\ 16\ 2.7\ 13\ 1\ 12\ 1\ -\ 13\ 0\ 13\ 1\ 9\ 1\ 33\ 4\ 229\ 3\ 06\ \times\ 10^{-6}\ 5\ 9\ 5\ 3\ 5\ 9\ 3\ 5\ 6\ 9\ 10\ 4\ 5\ 5\ 9\ 5\ 3\ 5\ 6\ 9\ 10\ 4\ 5\ 5\ 9\ 1\ 1\ 1\ 1\ 1\ 1\ 1\ 1\ 1\ 1\ 1\ 1\ 1\$		13 1 12 2 - 13 0 13 2	91 104.13	$3.02 \times 10^{-6}$	104.7
$ \begin{array}{c} 13\ 11\ 21\ -13\ 01\ 31\ \\ 6\ 34\ 1\ -7\ 26\ 2\ \\ 91\ 344\ 243\ 5\ .69\ \times10\ ^{4}\ 5\ .69\ \times10\ ^{4}\ 5\ .93\ .35\ \times10\ ^{-6}\ 6\ .40\ .40\ .40\ .40\ .40\ .40\ .40\ .40$		18 2 16 0 - 18 2 17 0	91 308.321	$5.09 \times 10^{-7}$	162.7
$ \begin{array}{c} 6 \ 3 \ 4 \ 1 - 7 \ 2 \ 6 \ 2 \\ 25 \ 8 \ 18 \ 0 - 26 \ 7 \ 19 \ 0 \\ 25 \ 8 \ 18 \ 0 - 26 \ 7 \ 19 \ 0 \\ 25 \ 8 \ 18 \ 0 - 26 \ 7 \ 19 \ 0 \\ 103 \ 308 \ 31 \ 1.11 \ 110^{-1} \ 6^{-1} \ 409.4 \\ 409.4 \\ 16 \ 4 \ 12 \ 0 - 17 \ 2 \ 15 \ 0 \\ 103 \ 308 \ 31 \ 1.11 \ 110^{-1} \ 6^{-1} \ 409.4 \\ 16 \ 4 \ 12 \ 0 - 17 \ 2 \ 15 \ 0 \\ 103 \ 308 \ 31 \ 1.11 \ 110^{-1} \ 6^{-1} \ 409.4 \\ 16 \ 4 \ 12 \ 0 - 17 \ 2 \ 15 \ 0 \\ 103 \ 308 \ 31 \ 1.11 \ 308 \ 1.11 \ 308 \ 408 \ 1.11 \ 308 \ 408 \ 1.11 \ 308 \ 408 \ 1.11 \ 308 \ 408 \ 1.11 \ 308 \ 408 \ 1.11 \ 308 \ 408 \ 1.11 \ 308 \ 408 \ 1.11 \ 308 \ 408 \ 1.11 \ 409 \ 409 \ 408$		13 1 12 1 - 13 0 13 1	91 334.229	$3.06 \times 10^{-6}$	104.6
$\begin{array}{c} 25 \ 8 \ 18 \ 0 \ - 26 \ 7 \ 19 \ 0 \\ 25 \ 8 \ 17 \ 0 \ - 26 \ 7 \ 20 \ 0 \\ 103 \ 303 \ 8.17 \ 1.11 \times 10^{-6} \ 409.4 \\ 16 \ 412 \ 0 \ - 17 \ 215 \ 0 \\ 103 \ 303 \ 8.431 \ 1.11 \times 10^{-6} \ 409.4 \\ 1.69 \times 10^{-8} \ 87.7 \\ \hline \\ $		6341-7262	91 344.243	$5.69 \times 10^{-8}$	59.3
$\begin{array}{c} 25 \ 8 \ 17 \ 0 \ - 26 \ 7 \ 20 \ 103 \ 308 \ 431 \ 1.11 \times 10^{-6} \ 409.4 \\ 16 \ 41 \ 20 \ - 17 \ 21 \ 5 \ 0 \ 103 \ 450.4 \ 1.69 \times 10^{-8} \ 151.2 \\ 11 \ 2 \ 10 \ 1 \ - 11 \ 10 \ 2 \ 103 \ 453.833 \ 1.35 \times 10^{-8} \ 87.7 \\ \hline \\ $		25 8 18 0 - 26 7 19 0	103 303.817	$1.11 \times 10^{-6}$	409.4
$\begin{array}{c} 164120-172150\\ 112101-111102\\ 103463.833\\ 1.35\times 10^{-8}\\ 87.7\\ \hline CHD_2CHO\\ 6152-5142\\ 103473.67\\ 3.75\times 10^{-9}\\ 40.1\\ 6060-5050\\ 103480.72\\ 3.72\times 10^{-9}\\ 17.4\\ \hline CH_3CH_2OH\\ 3913271-3814250\\ 90616.41\\ 4.90\times 10^{-7}\\ 916.5\\ 393361-394360\\ 90634.74\\ 5.11\times 10^{-6}\\ 728.3\\ 471462-460461\\ 90673.782\\ 1.70\times 10^{-8}\\ 916.6\\ 471462-460461\\ 90674.571\\ 1.70\times 10^{-8}\\ 916.6\\ 471462-460461\\ 90674.571\\ 1.70\times 10^{-8}\\ 916.6\\ 472462-461461\\ 9074.571\\ 1.70\times 10^{-8}\\ 916.6\\ 472462-461461\\ 90674.571\\ 1.70\times 10^{-8}\\ 916.6\\ 472462-460461\\ 9074.571\\ 1.70\times 10^{-8}\\ 916.6\\ 472404040\\ 193657\\ 1.30\times 10^{-7}\\ 921.5\\ 2812162-2911192\\ 90736.577\\ 1.33\times 10^{-7}\\ 921.5\\ 1422.202211930\\ 90947.962\\ 6.04\times 10^{-8}\\ 694.1\\ 212012-211920\\ 90947.962\\ 6.04\times 10^{-8}\\ 694.1\\ 212012-211920\\ 90947.962\\ 6.04\times 10^{-8}\\ 694.1\\ 212012-211920\\ 90947.962\\ 6.04\times 10^{-8}\\ 694.1\\ 212012-211930\\ 90947.962\\ 6.04\times 10^{-8}\\ 812.1\\ 251.5\\ 25242-24321\\ 90992.97\\ 8.40\times 10^{-8}\\ 432.1\\ 142132-133102\\ 90992.97\\ 8.40\times 10^{-8}\\ 432.1\\ 142132-133102\\ 90992.97\\ 8.40\times 10^{-8}\\ 432.1\\ 142132-133102\\ 90992.97\\ 8.40\times 10^{-8}\\ 432.1\\ 142132-131201\\ 91007.739\\ 991\times 10^{-7}\\ 272.8\\ 2511152-2610162\\ 91204.078\\ 8.20\times 10^{-7}\\ 424.7\\ 2511142-2610172\\ 91204.078\\ 8.20\times 10^{-7}\\ 928.1-8903\\ 318.623-10021\\ 9132886\\ 8.00\times 10^{-8}\\$		25 8 17 0 - 26 7 20 0	103 308.431	$1.11 \times 10^{-6}$	409.4
$\begin{array}{c} 112\ 110\ 1.1\ 110\ 2 & 103\ 403\ 833\ 1.35\times 10^{-8}\ 87.7 \\ \hline 112\ 101\ .1\ 111\ 102\ 103\ 463\ 833\ 1.35\times 10^{-8}\ 47.7 \\ \hline CHD_2CHO\ 6\ 15\ 2.5\ 14\ 2 & 103\ 473\ 67\ 3.75\times 10^{-9}\ 40.1 \\ 6\ 0\ 6\ 0\ .5\ 0\ 5\ 0 & 103\ 480\ .7\ 3.75\times 10^{-9}\ 40.1 \\ \hline 6\ 0\ 6\ 0\ .5\ 0\ 5\ 0 & 103\ 480\ .7\ 3.75\times 10^{-9}\ 17.4 \\ \hline CH_3CH_2OH\ 39\ 13\ 27\ 1\ .38\ 14\ 25\ 0 & 90\ 616\ .41\ 4\ .90\times 10^{-7}\ 916\ .5 \\ 39\ 3\ 36\ 1\ .39\ 43\ 6\ 0 & 90\ 634\ .7\ 4\ 5\ .11\times 10^{-6}\ 728.3 \\ 47\ 1\ 46\ 2\ .4\ 6\ 1\ 46\ 1\ 90\ 673\ .81\ 6\ 3.95\times 10^{-8}\ 916\ .6 \\ \hline 47\ 2\ 46\ 2\ .4\ 6\ 14\ 6\ 1\ 90\ 673\ .81\ 6\ 3.95\times 10^{-8}\ 916\ .6 \\ \hline 47\ 2\ 46\ 2\ .4\ 6\ 14\ 6\ 1\ 90\ 673\ .81\ 6\ 3.95\times 10^{-8}\ 916\ .6 \\ \hline 47\ 2\ 46\ 2\ .4\ 6\ 14\ 6\ 1\ 90\ 674\ .5\ 1\ .1\ 70\ ^{-8}\ 916\ .6 \\ \hline 47\ 2\ 46\ 2\ .4\ 6\ 14\ 6\ 1\ 90\ 674\ .5\ 1\ .1\ 70\ ^{-8}\ 916\ .6 \\ \hline 47\ 2\ 46\ 2\ .4\ 6\ 14\ 6\ 1\ 90\ 674\ .5\ 1\ .7\ .7\ ^{-8}\ 916\ .6 \\ \hline 47\ 2\ 46\ 2\ .4\ 6\ 14\ 6\ 1\ 90\ 674\ .5\ 1\ .7\ .7\ ^{-8}\ 916\ .6 \\ \hline 47\ 2\ 46\ 2\ .4\ 6\ 14\ 6\ 1\ 90\ 674\ .5\ 1\ .7\ .7\ ^{-8}\ 916\ .6 \\ \hline 47\ 2\ 46\ 2\ .4\ 0\ 46\ 1\ 90\ 674\ .5\ 1\ .7\ .7\ ^{-8}\ 916\ .6 \\ \hline 47\ 2\ 46\ 2\ .4\ 0\ 46\ 1\ 90\ 674\ .5\ 1\ .7\ .7\ .7\ .7\ .7\ .7\ .7\ .7\ .7\ .7$		16 4 12 0 - 17 2 15 0	103 450 4	$1.69 \times 10^{-8}$	151.2
$\begin{array}{c c c c c c c c c c c c c c c c c c c $		11 2 10 1 - 11 1 10 2	103 463 833	$1.05 \times 10^{-8}$	87.7
$\begin{array}{c} \text{G1D}_2\text{G1D} & \text{G1D}_2\text{G1D} & \text{G1D}_3\text{G1} & \text{G1D}_3\text{G1D}_3\text{G1} & \text{G1D}_3\text{G1} & \text{G1D}_3\text{G1}$	CHD <sub>2</sub> CHO	6152-5142	103 473 67	$\frac{1.55 \times 10}{3.75 \times 10^{-9}}$	40.1
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	endzenio	6061-5051	103 476 11	$3.72 \times 10^{-9}$	17.4
$\begin{array}{c c c c c c c c c c c c c c c c c c c $		6060-5050	103 480 72	$3.72 \times 10^{-9}$	17.1
$\begin{array}{c} 39 \ 13 \ 26 \ 1 & 38 \ 14 \ 24 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ $	CH2CH2OH	39 13 27 1 - 38 14 25 0	90.616.41	$\frac{3.72 \times 10}{4.90 \times 10^{-7}}$	916.5
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	onyonzon	39 13 26 1 - 38 14 24 0	90 616 41	$4.90 \times 10^{-7}$	916.5
$\begin{array}{c} 371462 - 461461 & 90673.782 & 1.70 \times 10^{-8} & 916.6 \\ 471462 - 460461 & 90673.782 & 1.70 \times 10^{-8} & 916.6 \\ 472462 - 461461 & 90674.536 & 3.95 \times 10^{-8} & 916.6 \\ 472462 - 460461 & 90674.571 & 1.70 \times 10^{-8} & 916.6 \\ 425381 - 435382 & 90701.878 & 1.88 \times 10^{-8} & 844.8 \\ 318242 - 306241 & 90724.54 & 2.48 \times 10^{-8} & 497.7 \\ 2812172 - 2911182 & 90736.557 & 7.33 \times 10^{-7} & 521.5 \\ 2812162 - 2911192 & 90736.557 & 7.33 \times 10^{-7} & 521.5 \\ 386331 - 397332 & 90809.192 & 1.68 \times 10^{-8} & 724.0 \\ 193161 - 192171 & 90824.709 & 5.78 \times 10^{-8} & 232.3 \\ 212012 - 211920 & 90947.962 & 6.04 \times 10^{-8} & 694.1 \\ 212022 - 211930 & 90947.962 & 6.04 \times 10^{-8} & 694.1 \\ 212022 - 211930 & 90947.962 & 6.04 \times 10^{-8} & 694.1 \\ 212022 - 211930 & 90981.716 & 5.24 \times 10^{-7} & 89.7 \\ 292271 - 297232 & 90992.97 & 8.40 \times 10^{-8} & 432.1 \\ 142132 - 133102 & 91007.739 & 9.91 \times 10^{-7} & 92.6 \\ 3610261 - 3511251 & 91030.969 & 3.31 \times 10^{-8} & 737.8 \\ 3610261 - 3511251 & 91030.969 & 3.31 \times 10^{-8} & 737.8 \\ 3610261 - 3511251 & 91030.969 & 3.31 \times 10^{-8} & 273.8 \\ 3610261 - 3511251 & 91030.969 & 3.31 \times 10^{-7} & 226.2 \\ 252242 - 243212 & 91058.798 & 1.52 \times 10^{-7} & 222.8 \\ 2511152 - 2610162 & 91204.078 & 8.20 \times 10^{-7} & 424.7 \\ 203171 - 203170 & 91219.35 & 5.52 \times 10^{-8} & 249.4 \\ 7260 - 7170 & 91241.609 & 7.12 \times 10^{-9} & 84.9 \\ 303282 - 310312 & 91250.931 & 1.83 \times 10^{-8} & 399.7 \\ 3816221 - 3816220 & 93183.533 & 6.06 \times 10^{-8} & 990.3 \\ 318232 - 306251 & 93145.898 & 3.66 \times 10^{-8} & 990.3 \\ 318232 - 306251 & 93145.898 & 3.66 \times 10^{-8} & 79.9 \\ 4231 - 4041 & 103320.469 & 1.28 \times 10^{-8} & 74.8 \\ 348261 - 348260 & 103380.759 & 6.84 \times 10^{-8} & 79.9 \\ 4231 - 4041 & 103320.469 & 1.28 \times 10^{-8} & 74.9 \\ 3510252 - 349250 & 93180.57 & 6.27 \times 10^{-9} & 655.1 \\ 3510252 - 349250 & 93180.57 & 6.27 \times 10^{-9} & 655.1 \\ 3510252 - 349250 & 93180.57 & 6.27 \times 10^{-9} & 655.1 \\ 348261 - 348270 & 103380.898 \times 10^{-8} & 74.9 \\ 37070 - 6160 & 103300.759 & 6.84 \times 10^{-8} & 79.9 \\ 4231 - 4041 & 103320.469 & 1.28 \times 10^{-8} & 74.9 \\ 376.3 & 7070 - 61600 $		39 3 36 1 - 39 4 36 0	90 634 74	$5.11 \times 10^{-6}$	728.3
$\begin{array}{c} 471462 - 460461 & 90673.816 & 3.95 \times 10^{-8} & 916.6 \\ 472462 - 460461 & 90674.536 & 3.95 \times 10^{-8} & 916.6 \\ 425381 - 435382 & 90701.878 & 1.88 \times 10^{-8} & 844.8 \\ 318242 - 306241 & 90724.54 & 2.48 \times 10^{-8} & 844.8 \\ 318242 - 306241 & 90736.55 & 7.33 \times 10^{-7} & 521.5 \\ 2812172 - 2911182 & 90736.571 & 7.33 \times 10^{-7} & 521.5 \\ 2812162 - 2911192 & 90736.571 & 7.33 \times 10^{-7} & 521.5 \\ 386331 - 397332 & 90809.192 & 1.68 \times 10^{-8} & 724.0 \\ 193161 - 192171 & 90824.709 & 5.78 \times 10^{-8} & 232.3 \\ 212012 - 211920 & 90947.962 & 6.04 \times 10^{-8} & 694.1 \\ 212022 - 211930 & 90947.962 & 6.04 \times 10^{-8} & 694.1 \\ 212022 - 211930 & 90947.962 & 6.04 \times 10^{-8} & 694.1 \\ 212012 - 1 - 32112219 & 909981.716 & 5.24 \times 10^{-7} & 89.7 \\ 292271 - 297232 & 90992.97 & 8.40 \times 10^{-8} & 737.8 \\ 3610261 - 3511251 & 91030.651 & 3.31 \times 10^{-8} & 737.8 \\ 3610261 - 3511251 & 91030.969 & 3.31 \times 10^{-8} & 737.8 \\ 3610261 - 3511251 & 91030.969 & 3.31 \times 10^{-8} & 737.8 \\ 3610261 - 3511251 & 91030.969 & 3.31 \times 10^{-8} & 737.8 \\ 3610261 - 3511251 & 91030.969 & 3.31 \times 10^{-8} & 737.8 \\ 3610261 - 3511251 & 91030.969 & 3.31 \times 10^{-8} & 737.8 \\ 3610261 - 3511251 & 91030.969 & 3.31 \times 10^{-8} & 737.8 \\ 3610261 - 3511251 & 91030.969 & 3.31 \times 10^{-8} & 737.8 \\ 3610261 - 3511251 & 91030.969 & 3.31 \times 10^{-8} & 737.8 \\ 3610261 - 3511251 & 91030.969 & 3.31 \times 10^{-8} & 737.8 \\ 3610261 - 3511251 & 91030.969 & 3.31 \times 10^{-8} & 737.8 \\ 3610261 - 3511251 & 91030.969 & 3.31 \times 10^{-8} & 737.8 \\ 3610261 - 3510262 & 91204.079 & 8.20 \times 10^{-7} & 424.7 \\ 2511142 - 2610172 & 91204.079 & 8.20 \times 10^{-7} & 424.7 \\ 2511142 - 2610172 & 91204.079 & 8.20 \times 10^{-7} & 424.7 \\ 2511252 - 349250 & 9138.533 & 6.6 \times 10^{-8} & 990.3 \\ 3816221 - 3816220 & 91332.886 & 8.06 \times 10^{-8} & 990.3 \\ 3816221 - 3816220 & 91332.886 & 8.06 \times 10^{-8} & 990.3 \\ 3816221 - 3816220 & 91332.886 & 8.06 \times 10^{-8} & 990.3 \\ 3816221 - 3816220 & 91332.886 & 8.06 \times 10^{-8} & 990.3 \\ 3816221 - 349250 & 93180.573 & 6.27 \times 10^{-9} & 655.1 \\ 256201 - 256200 & 103300.759 & 6.84 \times 10^{-8} & 79.9 \\ 4231 - 4041 & $		47 1 46 2 - 46 1 46 1	90 673 782	$1.70 \times 10^{-8}$	916.6
$\begin{array}{c} 47\ 2\ 46\ 2\ -\ 46\ 1\ 46\ 1\ 90\ 674.536\ 5.95\ \times\ 10^{-8}\ 916.6\\ 47\ 2\ 46\ 2\ -\ 46\ 0\ 46\ 1\ 90\ 674.571\ 1.70\ \times\ 10^{-8}\ 916.6\\ 42\ 5\ 38\ 1\ -\ 43\ 5\ 38\ 2\ 90\ 701.878\ 1\ .88\ \times\ 10^{-8}\ 844.8\\ 31\ 8\ 24\ 2\ .30\ 6\ 24\ 1\ 90\ 724.54\ 2\ .48\ \times\ 10^{-8}\ 844.8\\ 31\ 8\ 24\ 2\ .30\ 6\ 24\ 1\ 90\ 724.54\ 2\ .48\ \times\ 10^{-8}\ 844.8\\ 31\ 8\ 24\ 2\ .30\ 6\ 24\ 1\ 90\ 724.54\ 2\ .48\ \times\ 10^{-8}\ 844.8\\ 31\ 8\ 24\ 2\ .30\ 6\ 24\ 1\ 90\ 724.54\ 2\ .48\ \times\ 10^{-8}\ 844.8\\ 31\ 8\ 24\ 2\ .30\ 6\ 24\ 1\ 90\ 724.54\ 2\ .48\ \times\ 10^{-8}\ 844.8\\ 31\ 8\ 24\ 2\ .30\ 6\ 24\ 1\ 90\ 724.54\ 2\ .48\ \times\ 10^{-8}\ 844.8\\ 31\ 8\ 24\ 2\ .30\ 6\ 24\ 1\ 90\ 724.54\ 2\ .48\ \times\ 10^{-8}\ 844.8\\ 31\ 8\ 24\ 2\ .30\ 6\ 24\ 1\ 90\ 736.55\ 7\ .33\ \times\ 10^{-7}\ 5\ 21.5\\ 28\ 12\ 16\ 2\ .29\ 11\ 19\ 2\ 90\ 736.57\ 7\ .33\ \times\ 10^{-8}\ 724.0\\ 19\ 31\ 6\ 1\ .41\ 19\ 2\ 19\ 1\ 90\ 90\ 947.962\ 6\ .04\ \times\ 10^{-8}\ 694.1\\ 21\ 20\ 2\ .2\ 11\ 9\ 2\ 0\ 90\ 947.962\ 6\ .04\ \times\ 10^{-8}\ 694.1\\ 21\ 20\ 2\ .2\ 11\ 9\ 2\ 0\ 90\ 947.962\ 6\ .04\ \times\ 10^{-8}\ 694.1\\ 21\ 20\ 2\ .2\ 11\ 9\ 2\ 0\ 90\ 9947.962\ 6\ .04\ \times\ 10^{-8}\ 694.1\\ 21\ 21\ 9\ 1\ .2\ 12\ 19\ 0\ 90\ 9947.962\ 6\ .04\ \times\ 10^{-8}\ 694.1\\ 21\ 21\ 9\ 1\ .2\ 12\ 19\ 0\ 90\ 9947.962\ 6\ .04\ \times\ 10^{-8}\ 694.1\\ 21\ 21\ 9\ 1\ .2\ 12\ 19\ 0\ 90\ 9947.962\ 6\ .04\ \times\ 10^{-8}\ 694.1\\ 21\ 21\ 9\ 1\ .2\ 13\ 10\ 2\ 90\ 90\ 9947.962\ 6\ .04\ \times\ 10^{-8}\ 694.1\ 21\ 21\ 9\ 1\ .2\ 13\ .1\ .2\ 14\ 1\ 91\ 030\ .651\ 3\ .31\ \times\ 10^{-8}\ 737.8\\ 36\ 10\ 26\ 1\ .3\ .1\ .1\ .4\ .2\ 12\ .1\ .4\ .2\ .2\ .2\ .2\ .2\ .2\ .2\ .2\ .2\ .2$		47 1 46 2 - 46 0 46 1	90.673.816	$3.95 \times 10^{-8}$	916.6
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		47 2 46 2 - 46 1 46 1	90 674 536	$3.95 \times 10^{-8}$	916.6
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		47 2 46 2 - 46 0 46 1	90 674 571	$1.70 \times 10^{-8}$	916.6
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		42 5 38 1 - 43 5 38 2	90 701 878	$1.88 \times 10^{-8}$	844.8
$\begin{array}{c} 31 \ 021 \ 2 \ 0211 \ 182 \\ 28 \ 1217 \ 2 \ -2911 \ 182 \\ 28 \ 1216 \ 2 \ -2911 \ 192 \\ 3161 \ -192 \ 171 \\ 90 \ 736.57 \\ 7.33 \times 10^{-7} \ 521.5 \\ 38 \ 6331 \ -397 \ 332 \\ 90 \ 809.192 \\ 1.68 \times 10^{-8} \ 724.0 \\ 193 \ 161 \ -192 \ 171 \\ 90 \ 824.709 \\ 5.78 \times 10^{-8} \ 232.3 \\ 21 \ 201 \ 2 \ -21 \ 192 \ 0 \\ 90 \ 947.962 \\ 6.04 \times 10^{-8} \ 694.1 \\ 21 \ 20 \ 2 \ -21 \ 193 \ 0 \\ 90 \ 947.962 \\ 6.04 \times 10^{-8} \ 694.1 \\ 21 \ 20 \ 2 \ -21 \ 193 \ 0 \\ 90 \ 947.962 \\ 6.04 \times 10^{-8} \ 694.1 \\ 21 \ 20 \ 2 \ -21 \ 193 \ 0 \\ 90 \ 947.962 \\ 6.04 \times 10^{-8} \ 694.1 \\ 21 \ 20 \ 2 \ -21 \ 193 \ 0 \\ 90 \ 947.962 \\ 6.04 \times 10^{-8} \ 694.1 \\ 21 \ 21 \ 91 \ -21 \ 21 \ 9 \ 0 \\ 90 \ 981.716 \\ 5.24 \times 10^{-7} \ 89.7 \\ 292 \ 271 \ -297 \ 23 \ 2 \\ 90 \ 992.97 \\ 8.40 \times 10^{-8} \ 432.1 \\ 14 \ 21 \ 32 \ -13 \ 31 \ 02 \\ 91 \ 907.739 \\ 9.91 \times 10^{-7} \ 92.6 \\ 36 \ 10 \ 271 \ -35 \ 11 \ 24 \ 1 \\ 91 \ 030.651 \\ 3.31 \times 10^{-8} \ 737.8 \\ 36 \ 10 \ 26 \ 1 \ -35 \ 11 \ 25 \ 1 \\ 91 \ 030.651 \\ 3.31 \times 10^{-8} \ 737.8 \\ 36 \ 10 \ 26 \ 1 \ -35 \ 11 \ 25 \ 1 \\ 91 \ 037.88 \\ 1.52 \times 10^{-7} \ 727.28 \\ 25 \ 24 \ 2 \ -24 \ 3 \ 21 \ 2 \\ 91 \ 058.798 \\ 1.52 \times 10^{-7} \ 424.7 \\ 25 \ 11 \ 15 \ 2 \ -26 \ 10 \ 16 \ 2 \\ 91 \ 204.078 \\ 8.20 \times 10^{-7} \ 424.7 \\ 20 \ 3171 \ -20 \ 3170 \\ 91 \ 219.35 \ 5.52 \times 10^{-7} \ 424.7 \\ 20 \ 3171 \ -20 \ 3170 \\ 91 \ 219.35 \ 5.52 \times 10^{-8} \ 499.3 \\ 31 \ 8 \ 23 \ 2 \ -30 \ 625 \ 1 \\ 91 \ 32.886 \ 8.06 \times 10^{-8} \ 990.3 \\ 31 \ 8 \ 23 \ 2 \ -30 \ 625 \ 1 \\ 91 \ 332.886 \ 8.06 \times 10^{-8} \ 990.3 \\ 31 \ 8 \ 23 \ 2 \ -30 \ 625 \ 1 \\ 93 \ 145.898 \ 3.66 \times 10^{-8} \ 990.3 \\ 31 \ 8 \ 23 \ 2 \ -30 \ 625 \ 1 \\ 93 \ 145.898 \ 3.66 \times 10^{-8} \ 990.3 \\ 31 \ 8 \ 23 \ 2 \ -30 \ 625 \ 1 \\ 93 \ 145.898 \ 3.66 \times 10^{-8} \ 990.3 \\ 31 \ 8 \ 23 \ 2 \ -30 \ 625 \ 1 \\ 34 \ 8 \ 26 \ 1 \ -34 \ 8 \ 26 \ 103 \ 381.264 \ 9.03 \times 10^{-9} \ 655.1 \\ 34 \ 8 \ 26 \ 1 \ -34 \ 8 \ 27 \ 0 \ 103 \ 385.983 \ 8.98 \times 10^{-9} \ 655.1 \\ 34 \ 8 \ 26 \ 1 \ -34 \ 8 \ 27 \ 0 \ 103 \ 385.983 \ 8.98 \times 10^{-9} \ 655.1 \\ 34 \ 8 \ 27 \ 1 \ -34 \ 8 \ 27 \ 0 \ 103 \ 385.990 \ 1$		31 8 24 2 - 30 6 24 1	90 724 54	$2.48 \times 10^{-8}$	497 7
$\begin{array}{c} 28 12 16 2 - 29 11 19 2 \\ 28 12 16 2 - 29 11 19 2 \\ 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 \\ 72 6 1 - 6 3 4 0 \\ 90 991.716 \\ 5.24 \times 10^{-8} \\ 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 \\ 36 10 26 1 - 35 11 25 1 \\ 91 030.969 \\ 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 \\ 36 10 26 1 - 35 11 25 1 \\ 91 030.969 \\ 3.31 \times 10^{-8} \\ 737.8 \\ 36 10 26 1 - 35 11 25 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} \\ 722.8 \\ 25 11 14 2 - 26 10 16 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 2241.609 \\ 7.12 \times 10^{-9} \\ 84.9 \\ 30 3 28 2 - 31 0 31 2 \\ 91 332.886 \\ 8.06 \times 10^{-8} \\ 990.3 \\ 38 16 23 1 - 38 16 22 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} \\ 990.3 \\ 31 8 23 2 - 30 6 25 1 \\ 93 145.898 \\ 3.66 \times 10^{-8} \\ 990.3 \\ 31 8 23 2 - 30 6 25 1 \\ 93 145.898 \\ 3.66 \times 10^{-8} \\ 990.3 \\ 31 8 23 2 - 30 6 25 1 \\ 93 145.898 \\ 3.66 \times 10^{-8} \\ 990.3 \\ 31 8 23 2 - 30 6 25 1 \\ 93 145.898 \\ 3.66 \times 10^{-8} \\ 990.3 \\ 31 8 23 2 - 30 6 25 1 \\ 93 145.898 \\ 3.66 \times 10^{-8} \\ 990.3 \\ 31 8 23 2 - 30 6 25 1 \\ 93 145.898 \\ 3.66 \times 10^{-8} \\ 990.3 \\ 31 8 23 2 - 30 6 25 1 \\ 93 145.898 \\ 3.66 \times 10^{-8} \\ 990.3 \\ 31 8 23 2 - 30 6 25 1 \\ 93 145.898 \\ 3.66 \times 10^{-8} \\ 990.3 \\ 31 8 23 2 - 30 6 25 1 \\ 93 145.898 \\ 3.66 \times 10^{-8} \\ 990.3 \\ 31 8 23 2 - 30 6 25 1 \\ 93 145.898 \\ 3.66 \times 10^{-8} \\ 990.3 \\ 31 8 23 2 - 30 6 25 1 \\ 93 145.898 \\ 3.66 \times 10^{-8} \\ 990.3 \\ 31 8 23 2 - 30 6 25 1 \\ 93 145.898 \\ 3.66 \times 10^{-8} \\ 990.3 \\ 31 8 23 2 - 30 6 25 1 \\ 93 145.898 \\ 3$		28 12 17 2 - 29 11 18 2	9073655	$7.33 \times 10^{-7}$	521.5
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		28 12 16 2 - 29 11 19 2	90736571	$7.33 \times 10^{-7}$	521.5
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		38 6 33 1 - 39 7 33 2	90 809 192	$1.68 \times 10^{-8}$	724.0
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		19 3 16 1 - 19 2 17 1	90 824 709	$5.78 \times 10^{-8}$	232.3
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		21 20 1 2 - 21 19 2 0	90 947 962	$6.04 \times 10^{-8}$	694 1
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		21 20 2 2 - 21 19 3 0	90 947 962	$6.04 \times 10^{-8}$	694 1
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		21 2 19 1 - 21 2 19 0	90 968 68	$7.21 \times 10^{-8}$	262.0
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		7261-6340	90 981 716	$5.24 \times 10^{-7}$	89.7
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		29 2 27 1 - 29 7 23 2	90 992 97	$8.40 \times 10^{-8}$	432.1
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		142132 - 133102	91 007 739	$9.91 \times 10^{-7}$	92.6
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		36 10 27 1 - 35 11 24 1	91 030 651	$3.31 \times 10^{-8}$	737.8
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		36 10 26 1 - 35 11 25 1	91 030 969	$3.31 \times 10^{-8}$	737.8
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		18 3 15 1 - 18 2 16 1	91 047 417	$5.81 \times 10^{-8}$	216.2
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		25 2 24 2 - 24 3 21 2	91 058 798	$1.52 \times 10^{-7}$	272.8
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		25 11 15 2 - 26 10 16 2	91 204 078	$8.20 \times 10^{-7}$	474 7
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		25 11 14 2 - 26 10 17 2	91 204 079	$8.20 \times 10^{-7}$	424.7
$7260 - 7170$ $91241.609$ $7.12 \times 10^{-9}$ $84.9$ $303282 - 310312$ $91250.931$ $1.83 \times 10^{-8}$ $399.7$ $3816221 - 3816220$ $91332.886$ $8.06 \times 10^{-8}$ $990.3$ $3816231 - 3816230$ $91332.886$ $8.06 \times 10^{-8}$ $990.3$ $318232 - 306251$ $93145.898$ $3.66 \times 10^{-8}$ $990.3$ $3150252 - 349250$ $93180.157$ $6.27 \times 10^{-9}$ $655.1$ $3510252 - 349260$ $93183.533$ $6.27 \times 10^{-9}$ $655.1$ $256201 - 256200$ $103300.62$ $4.91 \times 10^{-9}$ $376.3$ $7070 - 6160$ $103330.759$ $6.84 \times 10^{-8}$ $79.9$ $4231 - 4041$ $103320.469$ $1.28 \times 10^{-8}$ $74.8$ $348261 - 348260$ $103381.264$ $9.03 \times 10^{-9}$ $635.1$ $9281 - 9191$ $103387.337$ $2.99 \times 10^{-8}$ $103.7$ $379281 - 379280$ $103403.957$ $2.12 \times 10^{-8}$ $745.6$		20 3 17 1 - 20 3 17 0	91 219 35	$5.20 \times 10^{-8}$	249.4
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		7260-7170	91 241 609	$7.12 \times 10^{-9}$	84.9
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		30 3 28 2 - 31 0 31 2	91 250 931	$1.83 \times 10^{-8}$	399.7
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		38 16 22 1 - 38 16 22 0	91 332 886	$8.06 \times 10^{-8}$	990.3
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		38 16 23 1 - 38 16 23 0	91 332 886	$8.06 \times 10^{-8}$	990.3
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		31 8 23 2 - 30 6 25 1	93 145 898	$3.66 \times 10^{-8}$	497 7
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		35 10 26 2 - 34 9 25 0	93 180 157	$6.27 \times 10^{-9}$	655 1
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		35 10 25 2 - 34 9 26 0	93 183 533	$6.27 \times 10^{-9}$	655.1
$7070-6160$ $103300.759$ $6.84 \times 10^{-8}$ $79.9$ $4231-4041$ $103320.469$ $1.28 \times 10^{-8}$ $74.8$ $348261-348260$ $103381.264$ $9.03 \times 10^{-9}$ $635.1$ $348271-348270$ $103385.983$ $8.98 \times 10^{-9}$ $635.1$ $9281-9191$ $103387.337$ $2.99 \times 10^{-8}$ $103.7$ $379281-379280$ $103403.957$ $2.12 \times 10^{-8}$ $745.6$		25 6 20 1 - 25 6 20 0	103 300 62	$4.91 \times 10^{-9}$	376 3
$4 2 3 1 - 4 0 4 1$ $103 320.469$ $1.28 \times 10^{-8}$ $74.8$ $34 8 26 1 - 34 8 26 0$ $103 381.264$ $9.03 \times 10^{-9}$ $635.1$ $34 8 27 1 - 34 8 27 0$ $103 385.983$ $8.98 \times 10^{-9}$ $635.1$ $9 2 8 1 - 9 1 9 1$ $103 387.337$ $2.99 \times 10^{-8}$ $103.7$ $37 9 28 1 - 37 9 28 0$ $103 404.936$ $2.12 \times 10^{-8}$ $745.6$		7070-6160	103 300 759	$6.84 \times 10^{-8}$	79.9
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		4231-4041	103 320 469	$1.28 \times 10^{-8}$	74.8
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		34 8 26 1 - 34 8 26 0	103 381 264	$9.03 \times 10^{-9}$	635.1
$9281 - 9191$ $103387.337$ $2.99 \times 10^{-8}$ $103.7$ $379281 - 379280$ $103403.957$ $2.12 \times 10^{-8}$ $745.6$ $379291 - 379280$ $103404.936 - 2.12 \times 10^{-8}$ $745.6$		34 8 27 1 - 34 8 27 0	103 385 983	$8.98 \times 10^{-9}$	635.1
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		9281-9191	103 387 337	$2.99 \times 10^{-8}$	103 7
37 0 20 1 - 37 0 20 0 103 103 103 103 107 2.12 × 10 745.0		37 9 28 1 - 37 9 28 0	103 403 957	$2.12 \times 10^{-8}$	745.6
JIJ 2J 1 - JIJ 2J U 10J 404.930 2.12 X 10 /43.0		37 9 29 1 - 37 9 29 0	103 404.936	$2.12 \times 10^{-8}$	745.6

# Table B.2: continued.

Species	Transition J K L M	Frequency (MHz)	$A_{ij}$ (s <sup>-1</sup> )	$E_{\rm up}$ (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
	6250-5240	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
	6250-6060	103 463.245	$5.33 \times 10^{-7}$	79.2
	6062-5052	103 480.355	$1.26 \times 10^{-8}$	17.5
	9180-8270	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
01120 0112 011	827-818	90 874.001	$3.63 \times 10^{-6}$	33.4
CH <sub>2</sub> CHDOH	46 6 40 - 45 9 37	90 764 508	$9.58 \times 10^{-8}$	946.6
011,0112 011	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
	551-642	91 219 103	$1.43 \times 10^{-7}$	38.3
	550-643	91 220 883	$1.13 \times 10^{-7}$ 1.43 × 10 <sup>-7</sup>	38.3
	1597 - 1688	01 220.005 01 235 784	$1.43 \times 10^{-7}$ 5 29 × 10 <sup>-7</sup>	183.0
	1596-1689	91 235.784	$5.27 \times 10^{-7}$	183.0
	1074 - 1165	91 200 202	$4.07 \times 10^{-7}$	Q6 2
	1074 - 1105 1073 - 1166	91 299.292	$4.07 \times 10^{-7}$	90.2
	724 725	91 299.390 102 415 2	$4.07 \times 10^{-6}$	90.2 22.5
	7 3 4 - 7 2 3	103 413.2	$0.01 \times 10^{-7}$	52.5 174.2
	20 2 19 - 19 3 10	103 499.033	$3.10 \times 10^{-6}$	1/4.2
	11 2 9 - 10 3 8	103 508.282	$\frac{2.08 \times 10^{-3}}{1.02 \times 10^{-7}}$	59.8
CH <sub>3</sub> OCHO	2/16/12/4 - 28/15/14/4	90 592.278	$1.03 \times 10^{-9}$	580.3
	23 3 20 0 - 24 2 23 0	90.649.201	$7.44 \times 10^{-7}$	173.2
	33 19 14 2 - 34 18 16 2	90707.602	$1.06 \times 10^{-7}$	570.2
	33 19 15 1 - 34 18 17 1	90719.908	$1.06 \times 10^{-7}$	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	90740.574	$1.06 \times 10^{-7}$	570.2
	9461-9362	90876.84	$6.31 \times 10^{-6}$	37.2
	17 3 14 5 - 17 2 15 5	90937.614	$1.13 \times 10^{-6}$	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
	9450-9360	91 356.766	$1.03 \times 10^{-6}$	37.2
	9452-9362	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
	10381-10192	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
	10380-10190	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
	8262-7252	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
	8260-7250	103 478.663	$1.52 \times 10^{-5}$	24.6

	Transition	England	A	E
Species		(MU <sub>7</sub> )	$A_{ij}$	$E_{\rm up}$
СЦ.ОСЦ.	$\frac{153120}{144110}$	00 880 262	$\frac{(8)}{1.02 \times 10^{-6}}$	(K) 122.5
CI130CI13	15 3 12 0 - 14 4 11 0 15 3 12 1 14 4 11 1	90 889.202	$1.02 \times 10^{-6}$	122.5
	15 3 12 1 - 14 4 11 1 15 3 12 5 - 14 4 11 5	90 892.20	$1.02 \times 10^{-6}$	122.5
	153123 - 144113 153123 - 144113	00 805 33	$1.02 \times 10^{-6}$	122.5
	6060 5150	90 895.55	$1.02 \times 10^{-6}$	122.5
	6061 5151	90 937.308	$3.03 \times 10^{-6}$	19.0
	6065 5155	90 938.107	$3.03 \times 10^{-6}$	19.0
	6063 5153	90 938.703	$3.03 \times 10^{-6}$	19.0
	5323 6423	90 958.707	$3.03 \times 10^{-7}$	19.0 36.1
	5323 - 0423 5321 6431	91 104.990	$1.13 \times 10^{-7}$	36.1
	5325 6435	91 175.205	$1.44 \times 10$ $3.45 \times 10^{-7}$	36.1
	5320 6430	01 184 531	$3.45 \times 10^{-7}$	36.1
	5320-0430	91 104.331	$3.40 \times 10^{-7}$	26.2
	5 2 5 - 0 4 5 5	91 105.051	$2.31 \times 10^{-7}$	26 1
	5 2 2 2 6 4 2 2	91 103.221	$2.02 \times 10^{-7}$	26.1
	5 5 5 5 - 04 2 5 5 2 2 1 6 4 2 1	91 223.214	$2.51 \times 10^{-7}$	26.1
	5335 6425	91 230.878	$2.02 \times 10^{-7}$	36.1
	5330 6420	91 231.309	$3.40 \times 10^{-7}$	26.1
	5330-0420 5331 6421	91 239.423	$3.47 \times 10^{-7}$	26.1
	5 3 3 3 6 4 3 3	91 240.890	$1.44 \times 10^{-7}$	26.2
	3 5 3 5 - 0 4 5 5 0 0 0 2 10 2 8 2	91 245.249	$1.10 \times 10^{-8}$	50.2 52.6
	9095-10385	91 343.406	$2.47 \times 10^{-8}$	52.6
	9095-10585	91 343.33	$2.47 \times 10^{-8}$	53.6
	9091 - 10381	01 358 263	$2.51 \times 10^{-8}$	53.6
	3030 - 10380	103 480 011	$2.33 \times 10^{-6}$	717.6
	32 12 20 3 - 33 13 20 3	103 409.911	$1.08 \times 10^{-6}$	717.0
	32 12 21 1 - 33 13 21 1	103 469.973	$1.08 \times 10^{-6}$	717.0
	32 12 20 0 - 33 13 21 0	103 490.039	$1.08 \times 10^{-6}$	717.0
	32 12 21 0 - 33 13 20 0	103 490.039	$1.08 \times 10^{-6}$	717.0
	32 12 20 5 - 33 13 21 5	103 490.137	$1.08 \times 10^{-6}$	717.0
	32 12 21 3 - 33 13 20 3	103 490.137	$1.08 \times 10^{-6}$	717.0
	32 12 20 1 - 33 13 20 1	103 490.221	$1.08 \times 10^{-6}$	717.0
СН СОСН	<u>32 12 21 3 - 33 13 21 3</u> <u>41 27 14 0 41 26 15 0</u>	00 505 107	$\frac{1.08 \times 10^{-5}}{2.62 \times 10^{-5}}$	709.7
CH <sub>3</sub> COCH <sub>3</sub>	4127140-4120150	90 595.197	$2.02 \times 10^{-5}$	106.7
	20 17 3 2 - 20 16 4 2	90 398.017	$1.28 \times 10^{-5}$	100.7
	20 17 4 2 - 20 10 3 2	90 030.940	$1.29 \times 10^{-5}$	100.7
	20 17 5 5 - 20 10 4 5	90 088.555	$1.29 \times 10^{-6}$	50.0
	$13 \ 5 \ 10 \ 1 - 13 \ 2 \ 11 \ 1$ $12 \ 4 \ 10 \ 1 - 12 \ 2 \ 11 \ 1$	90 090.137	$9.47 \times 10^{-6}$	50.0
	0722 8802	90 090.212	$9.47 \times 10^{-7}$	29.9
	9723-0003 271081 2718101	90 808.887	$4.03 \times 10^{-7}$	315.8
	27 19 8 1 - 27 18 10 1	90 812.049	$0.42 \times 10^{-6}$	18.5
	12 2 10 2 - 12 1 11 2 12 3 10 2 - 12 2 11 2	90 841 17	$7.02 \times 10^{-6}$	40.5
	$12 \ 5 \ 10 \ 2 - 12 \ 2 \ 11 \ 2$	90 841.14	$7.02 \times 10^{-6}$	40.5
	12 2 10 3 - 12 1 11 3	90 841.209	$7.02 \times 10^{-6}$	48.3
	$12 \ 5 \ 10 \ 5 \ - \ 12 \ 2 \ 11 \ 5$ $12 \ 3 \ 10 \ 0 \ 12 \ 2 \ 11 \ 0$	90 841.217	$7.02 \times 10^{-6}$	40.J 50.9
	$13 \ 5 \ 10 \ 0 - 13 \ 2 \ 11 \ 0$ $12 \ 4 \ 10 \ 0$ $12 \ 2 \ 11 \ 0$	90 842.133	$9.32 \times 10^{-6}$	50.0
	13 4 100 - 13 3 110	90 842.19	$9.33 \times 10^{-5}$	J9.8
	201741-201031	90 833.834	$1.29 \times 10^{-7}$	180.7
	13071-12941	908/9.430	$1.37 \times 10^{-5}$	10.5
	1 3 3 3 - 0 4 4 3	90 004./03	$2.10 \times 10^{-5}$	19.7
	1 3 3 2 = 0 2 4 2 2017 21 2016 41	90 889.338	$2.10 \times 10^{-5}$	19./ 102 0
	201/31-201041	90927.480	$1.29 \times 10^{-5}$	180.8
	20 19 8 3 - 20 18 9 3	90930.919	$1.03 \times 10^{-5}$	290.2
	/ 3 5 1 - 6 2 4 1	90 936.196	$2.10 \times 10^{-5}$	19.0
	25 12 11 2 - 25 11 12 2	90 94 / .328	$2.04 \times 10^{-5}$	218.4
	25 12 11 5 - 25 11 12 5	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.

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Table B.2:	continued.
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Species	Transition	Frequency	$A_{ij}$	$E_{\rm up}$
	<u>73 12 11 1 - 23 11 12 1</u>	90 964 992	$\frac{(3)}{2.04 \times 10^{-5}}$	218.4
	9733-8813	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
	7350-6240	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
	9721-8801	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
	9643-8713	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
	8531-8261	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	95400-87100	90 619.38	$1.29 \times 10^{-8}$	40.6
5	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	90716.134	$2.96 \times 10^{-9}$	496.3
	35 12 23 0 2 - 34 15 20 0 1	90716.134	$1.12 \times 10^{-8}$	496.3
	35 12 23 0 2 - 34 14 20 0 1	90716.15	$2.96 \times 10^{-9}$	496.3
	35 13 23 0 2 - 34 14 20 0 1	90716.15	$1.12 \times 10^{-8}$	496.3
	86200-84500	90727.049	$2.18 \times 10^{-8}$	34.4
	63401-52302	90757.201	$4.46 \times 10^{-6}$	17.0
	137700-129300	90 762.796	$2.50 \times 10^{-9}$	78.4
	93600-84400	90771.09	$2.25 \times 10^{-9}$	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
	86200-77000	90 901.78	$1.30 \times 10^{-7}$	34.4
	25 13 13 0 0 - 24 16 8 0 0	90917.361	$3.12 \times 10^{-9}$	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
	159600-1412200	90 983.691	$3.65 \times 10^{-9}$	108.9

Creation	Turnetition	<b>E</b>	4	F
Species	I K I M	(MHz)	$A_{ij}$ (s <sup>-1</sup> )	$E_{\rm up}$ (K)
	44 28 16 0 0 - 44 27 17 0 0	90.987.155	$\frac{(3)}{7.54 \times 10^{-6}}$	901.4
	43102-32201	91 024.622	$1.97 \times 10^{-6}$	9.4
	75200-73500	91 062.482	$1.18 \times 10^{-8}$	26.6
	86200-83500	91 071.232	$1.01 \times 10^{-7}$	34.4
	128500-1110200	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
	167900-1671000	91 104.88	$7.50 \times 10^{-7}$	115.2
	167900-1661000	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
	75200-72500	91 145.635	$5.62 \times 10^{-8}$	26.6
	97201-95502	91 159.53	$5.66 \times 10^{-8}$	42.9
	168900-1671000	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
	84400-76200	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
	63300-54200	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
	167902-1671001	91 372.165	$7.96 \times 10^{-7}$	115.0
	167902-1661001	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
	53300-41300	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	$8.93 \times 10^{-0}$	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	$2.84 \times 10^{-6}$	242.8
	30 20 11 0 0 - 30 19 12 0 0	103 402.047	$8.44 \times 10^{-9}$	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	$2.41 \times 10^{-7}$	531.8
	42200-31300	103 412.258	$5.21 \times 10^{-9}$	9.3
	18 14 5 00 - 1/ 16 2 0 0	103 452.707	$1.38 \times 10^{-6}$	163.5
	64201-54102	103 468.297	$2.68 \times 10^{-7}$	19.3
	15 5 10 0 1 - 15 5 11 0 2	103 469.421	9.90 × 10 ′	94.9
	15 5 10 0 1 - 15 4 11 0 2	103 469.491	$4.83 \times 10^{-6}$	94.9
	15 0 10 0 1 - 15 5 11 0 2	1034/1.5	$4.83 \times 10^{-7}$	94.9
	15 0 10 0 1 - 15 4 11 0 2	1034/1.57	$9.90 \times 10^{-9}$	94.9
	34 24 11 00 - 33 27 600	103 481.533	$2.07 \times 10^{-7}$	333.7
	42200-30300	105 480.552	1.19 X 10 '	9.3

Table B.2: continued.

Species	Transition	Frequency (MHz)	$A_{ij}$	$E_{\rm up}$
СН-ОНСНО	11.2.10 - 11.1.11	90 591 344	$\frac{(3)}{5.85 \times 10^{-6}}$	38.2
	11210-11111	90 785 464	$5.65 \times 10^{-6}$	8.0
	422-515 11/18 11/30	00 022 214	$1.24 \times 10^{-5}$	46 5
	32 11 22 31 12 10	90 922.214	$1.24 \times 10^{-6}$	368.0
	32 11 22 - 51 12 19	90 940.220	$2.43 \times 10^{-6}$	368.0
	A3 16 28 A2 17 25	01 277 8/10	$2.43 \times 10^{-6}$	682.0
	43 16 27 42 17 25	91 277.049	$2.30 \times 10^{-6}$	682.0
	43 10 27 - 42 17 20	102 201 285	$2.30 \times 10^{-5}$	28.2
	10010 - 919 15412 15212	103 391.203	$2.79 \times 10^{-5}$	20.5
	40 10 21 48 20 28	00.623.608	$\frac{1.78 \times 10}{2.17 \times 10^{-6}}$	801.0
ch20hch0	49 19 31 - 48 20 28	90 623 7	$2.17 \times 10^{-6}$	801.0
	23 5 18 23 <i>A</i> 10	90.629.1	$2.17 \times 10^{-5}$	1717
	23 5 18 - 25 + 19	90 029.132	$1.09 \times 10^{-5}$	100.0
	24 0 18 - 24 5 19	90 745.085	$1.63 \times 10^{-6}$	190.0 546.0
	33 20 14 34 19 10	90 765 157	$1.13 \times 10^{-6}$	546.9
	55 20 14 - 54 19 15 6 4 3 7 1 6	90 703.137	$1.13 \times 10^{-8}$	21.1
	043 - 710 23 3 20 24 2 23	90 791.284	$1.47 \times 10$ 7.05 × 10 <sup>-8</sup>	161.2
	$23 \ 3 \ 20 \ - \ 24 \ 2 \ 23$	90 855.954	$7.93 \times 10^{-9}$	101.2
	12 5 10 - 12 1 11 17 3 14 17 2 15	01 123 470	$9.70 \times 10^{-5}$	40.5
	17514 - 17215 19125 10129	91 125.479	$1.24 \times 10$ 7 50 × 10 <sup>-7</sup>	95.1
	18 13 6 10 12 7	91 151.742	$7.59 \times 10^{-7}$	194.7
	25.6.10 25.5.20	91 131.742	$1.39 \times 10^{-5}$	204.6
	23019 - 23320 1240 12310	91 230.931	$1.00 \times 10^{-5}$	204.0
	12 + 9 - 12 - 510 0.7.3 - 8.7.2	103 285 806	$1.20 \times 10^{-7}$	53.0
	973 - 872 072 - 871	103 285.890	$1.03 \times 10^{-7}$	53.9
	<i>3 1 2</i> - 0 <i>7 1</i> 37 13 25 36 14 22	103 203.9	$1.03 \times 10$ $3.52 \times 10^{-6}$	180.6
	37 13 24 36 14 22	103 349.428	$3.52 \times 10^{-6}$	489.0
	064 863	103 420 473	$3.32 \times 10^{-7}$	462
	963 862	103 420.473	$2.33 \times 10^{-7}$	46.2
	26 8 18 25 9 17	103 420.752	$2.33 \times 10^{-6}$	233.1
	52 8 44 - 53 7 47	103 468 404	$2.65 \times 10^{-7}$	235.1 815.0
СНДОНСНО	854-753	90 593 937	$\frac{2.00 \times 10}{1.71 \times 10^{-7}}$	33.1
end offente	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
	853-752	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
	836-735	90 678.44	$2.41 \times 10^{-7}$	24.5
	46 8 39 - 47 5 42	90679.401	$1.48 \times 10^{-7}$	625.6
	17 3 14 - 17 2 15	90722.053	$1.16 \times 10^{-5}$	91.2
	20 15 5 - 21 14 8	90728.937	$6.15 \times 10^{-7}$	236.2
	20 15 6 - 21 14 7	90728.937	$6.15 \times 10^{-7}$	236.2
	23 5 18 - 23 4 19	90751.425	$1.59 \times 10^{-5}$	168.3
	909-818	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
	845-744	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
	844-743	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	$2.36\times10^{-7}$	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

Species	Transition	Frequency	$A_{ij}$	$E_{up}$
	JKLM	(MHz)	(s <sup>-1</sup> )	(K)
	10 10 0 - 11 9 3	91 198.912	$1.11 \times 10^{-7}$	84.2
	919-818	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
$aGg-(CH_2OH)_2$	8171-7160	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	90675.102	$5.45 \times 10^{-8}$	88.0
	32 11 21 0 - 31 12 19 1	90675.776	$1.02 \times 10^{-7}$	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	90701.431	$1.30 \times 10^{-7}$	513.0
	33 22 12 0 - 34 21 13 0	90701.431	$1.30 \times 10^{-7}$	513.0
	26 4 22 0 - 26 4 23 1	90726.496	$8.82 \times 10^{-7}$	184.8
	14 5 10 0 - 14 4 11 0	90731.469	$1.99 \times 10^{-6}$	64.0
	15 5 11 0 - 15 4 12 0	90752.358	$2.03 \times 10^{-6}$	71.4
	53 10 43 0 - 53 10 44 1	90785.844	$7.06 \times 10^{-7}$	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	90839.672	$1.60 \times 10^{-7}$	513.4
	33 22 12 1 - 34 21 13 1	90839.672	$1.60 \times 10^{-7}$	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	90864.536	$1.26 \times 10^{-7}$	460.0
	31 21 11 0 - 32 20 12 0	90864.536	$1.26 \times 10^{-7}$	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	91041.27	$8.54 \times 10^{-6}$	494.3
	12580-12490	91.067.16	$1.92 \times 10^{-6}$	50.7
	12581-12491	91076.809	$2.13 \times 10^{-6}$	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
	2/1980-2818110	91 182.665	$1.14 \times 10^{-7}$	362.9
	2/1990-2818100	91 182.665	$1.13 \times 10^{-7}$	362.9
	14 3 11 1 - 13 4 10 1	91 186.341	$0.58 \times 10^{-7}$	57.4
	10 3 14 1 - 15 4 12 0	91213.836	$1.50 \times 10^{-7}$	/1.5
	14 3 11 0 - 13 4 10 0	91 224.675	$4.15 \times 10^{-7}$	5/.1
	28 9 20 0 - 27 10 18 1	91 234.81	$1.11 \times 10^{-7}$	239.8
	10550-10460	91 244.026	$1.81 \times 10^{-6}$	39.3
	10551-10461	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.

Table B.2:	continued.
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Species	Transition	Frequency (MHz)	$A_{ij}$ (s <sup>-1</sup> )	$E_{\rm up}$ (K)
	27 19 9 1 - 28 18 10 1	91 302.508	$\frac{(3^{-7})}{1.39 \times 10^{-7}}$	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
0 0 0 2 /2	9541-9451	90 625.64	$3.63 \times 10^{-6}$	34.2
	9540-9450	90 637.706	$3.50 \times 10^{-6}$	34.1
	22 6 17 0 - 22 5 17 1	90710.878	$3.12 \times 10^{-6}$	141.6
	9551-9461	90750.006	$3.54 \times 10^{-6}$	34.2
	9550-9460	90761.349	$3.62 \times 10^{-6}$	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
	8531-8441	90 862.788	$3.34 \times 10^{-6}$	29.8
	8530-8440	90 874.028	$3.28 \times 10^{-6}$	29.7
	8541-8451	90 911.505	$3.31 \times 10^{-6}$	29.8
	8540-8450	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
	7521-7431	91 016.495	$2.96 \times 10^{-6}$	25.9
	7520-7430	91 027.312	$2.92 \times 10^{-6}$	25.8
	7531-7441	91 032.962	$2.95 \times 10^{-6}$	25.9
	7530-7440	91 043.681	$2.93 \times 10^{-6}$	25.8
	4321-3211	91 101.828	$4.93 \times 10^{-6}$	9.3
	6511-6421	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
	6521-6431	91 117.61	$2.39 \times 10^{-6}$	22.5
	6510-6420	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
	6520-6430	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
	5501-5411	91 170.801	$1.52 \times 10^{-6}$	19.5
	5511-5421	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
	5500-5410	91 181.28	$1.50  imes 10^{-6}$	19.5
	5510-5420	91 182.189	$1.50  imes 10^{-6}$	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

Species	Transition	Frequency	A <sub>ij</sub>	Eup
	JKLM	(MHz)	$(s^{-1})$	(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
	9281-8270	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
	9451-8440	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
	10471-9460	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	514-515	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	1165-1156	90 842.056	$8.21 \times 10^{-6}$	137.2
2 1	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	955-936	90 667.609	$1.17 \times 10^{-7}$	83.6
2 5 -	725-726	90 683.057	$9.45 \times 10^{-8}$	48.3
	725-716	90710.475	$4.70 \times 10^{-6}$	48.3
	10 8 2 - 10 7 3	90781.87	$6.42 \times 10^{-6}$	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	$2.03 \times 10^{-8}$ 2 49 × 10 <sup>-8</sup>	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	$1.01 \times 10^{-6}$	153.8
	21 7 13 - 22 6 10	103 385 42	$1.23 \times 10^{-6}$ $1.23 \times 10^{-6}$	153.8
	60 4 57 59 5 54	103 / 17 1/7	$1.23 \times 10^{-7}$	802.3
HOCH CN	$\frac{00457 - 59554}{382360 - 301300}$	00 507 603	$\frac{2.03 \times 10}{5.26 \times 10^{-8}}$	338.5
noch2ch	25 2 23 0 25 1 24 0	90 597.005	$5.20 \times 10^{-6}$	151.6
	252250-251240 184140 183161	90 619.344	$4.38 \times 10^{-6}$	08.0
	104140 - 105101 268200 - 277200	90 055.579	$2.67 \times 10^{-6}$	90.0 202 0
	36 8 38 0 - 37 7 31 0	90733.122	$1.17 \times 10^{-6}$	202.0 202.0
	JU 0 20 U - J / JI U 10 4 15 0 10 2 17 1	90/3/.103	$1.1 / X IU^{\circ}$	303.0 104 4
	194130-1931/1	90 808.881	$2.00 \times 10^{-8}$	100.4
	49 5 45 1 - 50 2 48 1	90.829.279	$\delta.33 \times 10^{-7}$	383.4
	25 4 19 1 - 24 2 22 1	90918.82	1.95 × 10 ′	149.9
	29 5 25 1 - 30 4 27 0	90932.471	$1.2/ \times 10^{-7}$	232.8
	23 2 21 0 - 23 1 23 1	90938.751	$8.9/ \times 10^{-7}$	129.5
	8081-8180	90 948.488	$0.84 \times 10^{-0}$	21.3
	8181-7260	90973.549	$8.01 \times 10^{-7}$	22.3

Table B.2: continued.

Table	<b>B</b> .2:	continued
raute	$\mathbf{D}, \mathbf{\Delta}, \mathbf{C}$	continucu

J K L M(MHz) $(s^{-1})$ (K)20 4 16 0 - 20 3 18 191 039.63 $2.87 \times 10^{-6}$ 115.342 2 40 0 - 41 4 37 091 089.387 $1.69 \times 10^{-7}$ 410.456 7 50 1 - 55 8 47 191 170.271 $1.30 \times 10^{-6}$ 780.449 5 45 0 - 50 2 48 091 212.431 $1.20 \times 10^{-7}$ 578.410 0 10 1 - 9 0 9 191 244.602 $2.25 \times 10^{-5}$ 29.635 6 30 1 - 36 5 32 091 280.978 $1.27 \times 10^{-6}$ 334.410 0 10 0 - 9 0 9 091 282.104 $2.27 \times 10^{-5}$ 24.229 2 27 1 - 29 2 28 191 307.51 $1.12 \times 10^{-7}$ 206.321 4 17 0 - 21 3 19 191 343.484 $2.87 \times 10^{-6}$ 124.634 3 32 0 - 33 4 29 093 175.688 $1.03 \times 10^{-6}$ 276.016 1 15 0 - 15 1 15 193 179.831 $4.57 \times 10^{-7}$ 62.830 9 21 0 - 31 8 23 193 190.634 $9.50 \times 10^{-7}$ 318.335 2 33 0 - 34 3 31 1103 318.063 $3.15 \times 10^{-6}$ 288.945 3 42 1 - 45 3 42 0103 318.12 $9.15 \times 10^{-6}$ 901.220 2 18 0 - 19 2 18 1103 352.311 $7.48 \times 10^{-8}$ 99.721 4 17 1 - 22 3 19 0103 421.493 $1.71 \times 10^{-6}$ 130.332 2 30 1 - 32 2 30 0103 402.141 $1.77 \times 10^{-6}$ 80.846 8 38 1 - 47 7 40 0103 440.794 $1.79 \times 10^{-6}$ 572.848 444 1 - 48 444 0103 506.105 $1.08 \times 10^{-7}$ 572.9NH2CHO15 3 12 - 16 1 1591 136.103 $4.85 \times 10^{-7}$ 757.220 5 16 - 21 4	Species	Transition	Frequency	A <sub>ij</sub>	$E_{\rm up}$
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		JKLM	(MHz)	$(s^{-1})$	(K)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		20 4 16 0 - 20 3 18 1	91 039.63	$2.87 \times 10^{-6}$	115.3
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		42 2 40 0 - 41 4 37 0	91 089.387	$1.69 \times 10^{-7}$	410.4
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		56 7 50 1 - 55 8 47 1	91 170.271	$1.30 \times 10^{-6}$	780.4
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$		49 5 45 0 - 50 2 48 0	91 212.431	$1.20 \times 10^{-7}$	578.4
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		10 0 10 1 - 9 0 9 1	91 244.602	$2.25 \times 10^{-5}$	29.6
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		35 6 30 1 - 36 5 32 0	91 280.978	$1.27 \times 10^{-6}$	334.4
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		10 0 10 0 - 9 0 9 0	91 282.104	$2.27 \times 10^{-5}$	24.2
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		29 2 27 1 - 29 2 28 1	91 307.51	$1.12 \times 10^{-7}$	206.3
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		21 4 17 0 - 21 3 19 1	91 343.484	$2.87 \times 10^{-6}$	124.6
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		34 3 32 0 - 33 4 29 0	93 175.688	$1.03 \times 10^{-6}$	276.0
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		16 1 15 0 - 15 1 15 1	93 179.831	$4.57 \times 10^{-7}$	62.8
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		30 9 21 0 - 31 8 23 1	93 190.634	$9.50 \times 10^{-7}$	318.3
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		30 9 22 0 - 31 8 24 1	93 190.64	$9.50 \times 10^{-7}$	318.3
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		35 2 33 0 - 34 3 31 1	103 318.063	$3.15 \times 10^{-6}$	288.9
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		45 3 42 1 - 45 3 42 0	103 318.312	$9.15 \times 10^{-8}$	482.2
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		59 9 51 1 - 58 10 49 0	103 334.357	$1.76 \times 10^{-6}$	901.2
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		59 9 50 1 - 58 10 48 0	103 341.424	$1.76 \times 10^{-6}$	901.2
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		20 2 18 0 - 19 2 18 1	103 352.311	$7.48 \times 10^{-8}$	99.7
$\begin{array}{c} 32\ 2\ 30\ 1-32\ 2\ 30\ 0 \\ 27\ 4\ 23\ 1-26\ 5\ 21\ 0 \\ 57\ 7\ 50\ 0-56\ 8\ 49\ 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 \\ \hline NH_2CHO \\ 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 \\ \hline CH_3SH \\ 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\ 399.789 \\ 5.79\ \times\ 10^{-7} \\ 133.6 \\ 8\ 0\ 8\ 0\ -\ 7\ 16\ 0 \\ 103\ 504.193 \\ 1.54\ \times\ 10^{-6} \\ 43.7 \\ 27\ 5\ 22\ -3\ -26\ 6\ 21\ -3 \\ 103\ 509.321 \\ 5.40\ \times\ 10^{-7} \\ 870.7 \\ \hline 27\ -5\ 23\ -3\ -26\ -6\ 21\ -3 \\ \hline 103\ 509.321 \\ 5.40\ \times\ 10^{-7} \\ 870.7 \\ \hline 870.7 \\ \ 870.7 \\ \hline 870.7 \\ \ 870.7 $		21 4 17 1 - 22 3 19 0	103 384.207	$1.71 \times 10^{-6}$	130.0
$\begin{array}{c} 27\ 4\ 23\ 1\ -\ 26\ 5\ 21\ 0 \\ 57\ 7\ 50\ 0\ -\ 56\ 8\ 49\ 0 \\ 103\ 421.493 \\ 1.71\ \times\ 10^{-6} \\ 195.2 \\ 57\ 7\ 50\ 0\ -\ 56\ 8\ 49\ 0 \\ 103\ 437.673 \\ 1.87\ \times\ 10^{-6} \\ 800.8 \\ 46\ 8\ 38\ 1\ -\ 47\ 7\ 40\ 0 \\ 103\ 440.794 \\ 1.79\ \times\ 10^{-6} \\ 572.8 \\ 48\ 4\ 44\ 1\ -\ 48\ 4\ 44\ 0 \\ 103\ 506.105 \\ 1.08\ \times\ 10^{-7} \\ 552.9 \\ \hline NH_2CHO \\ 15\ 3\ 12\ -\ 16\ 1\ 15 \\ 91\ 136.103 \\ 4.85\ \times\ 10^{-8} \\ 149.5 \\ 36\ 5\ 32\ -\ 35\ 6\ 29 \\ 103\ 296.485 \\ 7.38\ \times\ 10^{-7} \\ 755.7 \\ 20\ 5\ 16\ -\ 21\ 4\ 17 \\ 103\ 446.144 \\ 7.16\ \times\ 10^{-7} \\ 288.6 \\ \hline CH_3SH \\ 1\ -\ 1\ 1\ 1\ -\ 0\ 0\ 0\ 1 \\ 90\ 637.359 \\ 7.97\ \times\ 10^{-7} \\ 5.8 \\ 12\ -\ 11\ 2\ 4\ -\ 11\ -\ 2\ 10\ 4 \\ 91\ 128.19 \\ 3.80\ \times\ 10^{-7} \\ 571.2 \\ 9\ 1\ 8\ 1\ -\ 9\ 0\ 9\ 1 \\ 103\ 399.789 \\ 5.79\ \times\ 10^{-7} \\ 133.6 \\ 8\ 0\ 8\ 0\ -\ 7\ 16\ 0 \\ 103\ 504.193 \\ 1.54\ \times\ 10^{-6} \\ 43.7 \\ 27\ 5\ 22\ -3\ -\ 26\ 6\ 20\ -3 \\ 103\ 508.935 \\ 5.40\ \times\ 10^{-7} \\ 870.7 \\ 27\ -5\ 23\ -3\ -\ 26\ -6\ 21\ -3 \\ 103\ 509.321 \\ 5.40\ \times\ 10^{-7} \\ 870.7 \\ \hline 870.7 \\ \ 870.7 \ \ 870.7 \ \ 870.7 \\ \ 870.7 \\ \ 870.7 \\ \ 870.7 \\ \ 870.7 \\ \ 870.7 \\ \ 870.7 \\ \ 870.7 \\ \ 870.7 \\ \ 870.7 \\ \ 870.7 \\ \ 870.7 \\ \ 870.7 \ \ 870.7 \\ \ 870.7 \\ \ 870.7 \\ \ 870.7 \ \ 870.7 \\ \ 870.7 \ \ 870.7 \\ \ 870.7 \ \ 870.7 \\ \ 870.7 \ \ 870.7 \\ \ 870.7 \ \ 870.7 \\ \ 870.7 \ \ 870.7 \ \ 870.7 \\ \ 870.7 \ \ 870.$		32 2 30 1 - 32 2 30 0	103 402.141	$1.77 \times 10^{-6}$	248.2
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		27 4 23 1 - 26 5 21 0	103 421.493	$1.71 \times 10^{-6}$	195.2
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		57 7 50 0 - 56 8 49 0	103 437.673	$1.87 \times 10^{-6}$	800.8
$\begin{array}{c c c c c c c c c c c c c c c c c c c $		46 8 38 1 - 47 7 40 0	103 440.794	$1.79 \times 10^{-6}$	572.8
$\begin{array}{c c c c c c c c c c c c c c c c c c c $		48 4 44 1 - 48 4 44 0	103 506.105	$1.08 \times 10^{-7}$	552.9
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	NH <sub>2</sub> CHO	15 3 12 - 16 1 15	91 136.103	$4.85 \times 10^{-8}$	149.5
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		36 5 32 - 35 6 29	103 296.485	$7.38 \times 10^{-7}$	755.7
$\begin{array}{c c c c c c c c c c c c c c c c c c c $		20 5 16 - 21 4 17	103 446.144	$7.16 \times 10^{-7}$	288.6
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	CH <sub>3</sub> SH	1 -1 1 1 - 0 0 0 1	90 637.359	$7.97 \times 10^{-7}$	5.8
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		12 -1 12 4 - 11 -2 10 4	91 128.19	$3.80 \times 10^{-7}$	571.2
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		9181-9091	103 389.812	$2.55 \times 10^{-6}$	61.0
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		12 3 9 1 - 13 2 11 1	103 399.789	$5.79 \times 10^{-7}$	133.6
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		8080-7160	103 504.193	$1.54 \times 10^{-6}$	43.7
27 -5 23 -3 - 26 -6 21 -3 103 509.321 5.40 × 10 <sup>-7</sup> 870.7		27 5 22 -3 - 26 6 20 -3	103 508.935	$5.40  imes 10^{-7}$	870.7
		27 -5 23 -3 - 26 -6 21 -3	103 509.321	$5.40 \times 10^{-7}$	870.7