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Rotational spectrum of deuterated and ^{15}N ethyl cyanides: CH_3CHDCN and CH_2DCH_2CN and of $CH_3CH_2C^{15}N$[⋆,⋆⋆]

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ABSTRACT

Context. Ethyl cyanide is an abundant molecule in hot molecular clouds. Its rotational spectrum is very dense and several hundreds of rotational transitions within the ground state have been identified in molecular clouds in the 40−900 GHz frequency range. Lines from ^{13}C isotopically substituted ethyl cyanide were identified in Orion.

Aims. To enable the search and the possible detection of other isotopologues of ethyl cyanide in interstellar objects, we have studied the rotational spectrum of deuterated ethyl cyanide: CH_2DCH_2CN (in-plane and out-of-plane) and CH_3CHDCN and the spectrum of ^{15}N substituted ethyl cyanide $CH_3CH_2C^{15}N$. Using these experimental data, we have searched for these species in Orion.

Methods. The rotational spectrum of each species in the ground state was measured in the microwave and millimeter-submillimeter wavelength range using a waveguide Fourier Transform spectrometer (8−17 GHz) and a source-modulated spectrometer employing backward-wave oscillators (BWOs) (150−260 and 580−660 GHz). More than 300 lines were identified for each species, for J values in the range 71−80 and K_a values in the range 28−31 depending on the isotopologues. The experimental spectra were analyzed using a Watson's Hamiltonian in the A-reduction.

Results. From the fitting procedure, accurate spectroscopic constants were derived for each of the species. These new sets of spectroscopic constants enable us to predict reliably the rotational spectrum (lines frequencies and intensities) in the 4−1000 GHz frequency range and for J and K_a up to 80 and 31, respectively. Combined with IRAM 30 m antenna observations of Orion, this experimental study allowed us to detect ^{15}N substituted ethyl cyanide $CH_3CH_2C^{15}N$ for the first time in Orion. The derived column density and rotational temperature are 10^{13} cm^{-2} and 150 K for the plateau and 3×10^{14} cm^{-2} and 300 K for the hot core. The deuterated species were searched for but were not detected. The upper limit to the column density of each deuterated isotopologues was 10^{14} cm^{-2}.

Key words. line: identification – methods: laboratory – molecular data – ISM: molecules – radio lines: ISM – submillimeter

1. Introduction

Ethyl cyanide, CH_3CH_2CN, is an asymmetric top molecule with a large dipole moment (μ_a = 3.85 D and μ_b = 1.23 D) that exhibits a dense and intense rotational spectrum. It is present in the densest parts of hot molecular cores, where it is proposed to form on dust grains. Several hundreds of lines of CH_3CH_2CN in the ground state have been observed towards hot cores such as Orion, Sgr B2 and W51 (Miao & Snyder 1997; Liu et al. 2001) but also toward low mass star-forming regions (Cazaux et al. 2003; Remijan & Hollis 2006). It has a high abundance of the order of 10^{15}–10^{17} cm^{-2} depending on the sources (Miao & Snyder 1997; Remijan et al. 2004; Remijan & Hollis 2006). Transitions from vibrationally excited ethyl cyanide have also been observed in Sgr B2 (Mehringer et al. 2004) and in W51 e2 (Demyk et al. 2008). Numerous lines from ^{13}C-substituted ethyl cyanide have been detected in Orion Irc2 (Demyk et al. 2007).

All of these observations show that the unidentified lines observed in spectral surveys of molecular clouds are partly due to transitions from known species in vibrationally excited states or from isotopologues of known species. The most promising carriers of these transitions are the so-called *interstellar weeds*, i.e. molecules, such as ethyl cyanide, which have a dense and intense rotational spectrum and/or low-frequency vibrational modes, such as methyl formate $HCOOCH_3$, dimethyl-ether CH_3OCH_3, or methanol CH_3OH. With the increase in sensitivity and frequency coverage that will be achieved with instruments such as HIFI onboard the Herschel Space Observatory and ALMA, the identification of these *U-lines* will become crucial to the search for new molecules but also to obtain important information about the physical and chemical conditions prevailing in the observed sources.

An enormous amount of experimental work must be undertaken to complete the actual knowledge of the rotational spectra

⋆ Full version of Tables 7 to 10 are only available in electronic form at the CDS via anonymous ftp to cdsarc.u-strasbg.fr (130.79.128.5) or via http://cdsweb.u-strasbg.fr/cgi-bin/qcat?J/A+A/493/565
⋆⋆ Tables 3 to 11 are only available in electronic form at http://www.aanda.org

of low-frequency vibrational mode and of the isotopologues of abundant interstellar molecules. When they exist, measurements are indeed often limited to low frequencies and therefore cannot be used to predict reliable line frequencies and intensities in the Herschel and ALMA frequency ranges.

In this context, following up our study on ^{13}C-substituted ethyl cyanide (Demyk et al. 2007), we present an experimental study of the rotational spectrum of deuterated ethyl cyanide, CH_2DCH_2CN in-plane, CH_2DCH_2CN out-of-plane, CH_3CHDCN, and ^{15}N substituted ethyl cyanide, $CH_3CH_2C^{15}N$. These species were studied 30 years ago by Mäder et al. (1973) and Heise et al. (1976). For each species, about 30 low-J ($J \leq 6$) rotational transitions were recorded and assigned in the 4−40 GHz frequency range. The rotational constants and quadrupole coupling constants derived from these studies were used to extend the measurements to higher frequency. The isotopologues synthesis and the experimental setup are described in Sect. 2. The analysis of the measured rotational transitions, the resulting spectroscopic parameters, and the prediction of rotational spectrum for each isotopologue in the 8−1000 GHz range are presented in Sect. 3. The detection of $CH_3CH_2C^{15}N$ in Orion and the search for the deuterated species is presented in Sect. 4.

2. Experimental setup

The deuterated ethyl cyanides, CH_2DCH_2CN and CH_3CHDCN, have been prepared from the corresponding ethyl iodides CH_2DCH_2I and CH_3CHDI (98 atom%, C/D/N isotopes, Pointe Claire, Canada) and normal potassium cyanide. $KC^{15}N$ (98 atom%, Aldrich, Taufkirchen, Germany) and normal ethyl iodide were used for the preparation of the ^{15}N-isotopologue. The potassium cyanide was dispersed in a solution of ethyl iodide in triethylene glycol and the mixture was stirred and heated slowly to 110 °C. Potassium cyanide and ethyl iodide were used in a molar ratio 1.25: 1.00, and the concentration of the ethyl iodide solution was 4 mol/l. Nitrogen was bubbled through the mixture and the ethyl cyanide was isolated in an ice-cooled trap. The yield of this modified Kolbe reaction (Organikum 1977; Mäder et al. 1973) was 75%. The product was distilled and controlled spectroscopically. The only detectable impurity was a small amount of the corresponding isonitrile.

In Kiel, the measurements in the centimeter-wave range were performed by means of waveguide Fourier-transform microwave-spectroscopy (Sarka et al. 1997). A spectrometer in the range of about 8−17 GHz was used, employing an oversized X-band sample cell with a rectangular waveguide of quadratic cross-section and 12 m length (Krüger et al. 1993). The experiments were carried out at ambient temperature and at gas pressures of ca. 0.1 Pa. Experimental transition frequencies were obtained from an analysis of the frequency-domain signals; these were derived following Fourier transformation of the transient emission signal, using a peak finder routine that determined line-center frequencies to an accuracy typically superior to 20 kHz, depending on the strength of the line. In the case of observed line splittings due to methyl internal rotation (AE-splittings) and/or the ^{14}N-nuclear quadrupole coupling, the experimental peak frequencies were corrected to obtain hypothetical unsplit line frequencies (without nuclear quadrupole hyperfine structure).

The millimeter spectra were recorded in Lille in the spectral range 150−250 and 580−660 GHz. The sources were Russian Istok backward-wave oscillators (BWO). They were phase locked on an harmonic from a HP synthesizer. Up to 250 GHz, the signal from the synthesizer was directly mixed onto a Russian planar Schottky diode with part of the signal from the BWO. From 500 GHz to 650 GHz, an active sextupler from millitech (75−100 GHz) and a Schottky planar diode placed in a parabolic structure (from Virginia Diodes Inc.) optimized for this range were used. The detector was an InSb liquid He-cooled bolometer from QMC. To improve the sensitivity of the spectrometer, the sources were frequency-modulated at 5 kHz. The absorption cell was a stainless steel tube (6 cm diameter, 110 cm long), and the pressure that we used during measurements was 2.6 Pa (26 μbar). The accuracy of isolated lines was superior to 30 kHz.

3. Spectral analysis and line predictions

Ethyl cyanide and its isotopologues are prolate asymmetric top molecules. The main isotopologue, CH_3CH_2CN, has a large dipole moment (μ_a = 3.83 D, μ_b = 1.23 D; Heise et al. 1976), which was used to calculate the lines intensities of the four studied isotopologues, since it was found that the rotation of the principal axes system upon isotopic substitution does not induce significant variation in the dipole moment. The experimental spectrum of each isotopologue is very dense and intense. It contains lines from the main isotopologue, which may be present as a trace in the samples. It also exhibits lines from the first low-frequency vibrationally excited states (the CH_3 torsion mode and the CCN bending mode). Consequently, some lines in the measured spectra are blended or distorted and are therefore not used in the analysis. ^{14}N-nuclear quadrupole coupling and the internal rotation of the CH_3 group introduce splitting of the lines. However, these effects were not taken into account in the analysis, since these splittings are not observed in the millimeter range, and in the microwave region the unsplit line frequencies are used when splitting is observed.

The spectral analysis is a step-by-step process with permanent interaction between measurements and theory. First of all, we used the spectroscopic parameters derived from previous experimental studies at low frequency (4−40 GHz) to provide a first prediction of the line positions at low frequency and for low J and K_a value for each species. We used the experimental work from Heise et al. (1976) and Mäder et al. (1976) for $CH_3CH_2C^{15}N$ and CH_2DCH_2CN, respectively. The quartic distortional constants missing (δ_J and δ_K) were fixed to the values of the normal species. In the absence of any experimental data, the rotational constants of CH_3CHDCN, were calculated using ab initio calculation at the level B3LYP/6-31G* with Gaussian 03 (Frisch et al. 2004). Based on these predictions, new lines were identified in new measurements performed in the 8−17 GHz range. All of the measured lines were then fitted to derive a new and more accurate set of spectroscopic constants. These constants were then used to derive a new prediction at higher frequency and for a higher value of J and K_a. New lines were measured and added to the fit step by step until the fit of the measured lines and the precision of the derived spectroscopic parameters were sufficiently good for a reliable prediction to be made for the desired frequency range and value of quantum numbers. For the fitting procedure of the measured lines and for the predictions, we have used a Watson's Hamiltonian using A-reduction in I^r representation (Watson 1977). The S reduction was also attempted but without significant improvement (as for the ^{13}C species, Demyk et al. 2007). The molecular parameters were determined by fitting the experimental frequencies using the iteratively re-weighted least squares fitting method (Hamilton 1992; Bakri et al. 2002). The objective of this method was to derive suitable weights using the residuals of a previous iteration. It had the advantage of being more robust than the

Table 1. Spectroscopic measurements of the ground vibrational state of CH_3CHDCN, CH_2DCH_2CN and $CH_3CH_2C^{15}N$.

	Number of measured lines		J max	K_a max	Standard
	8–39 GHz	150–660 GHz			deviation[a] (kHz)
CH_2DCH_2CN in-plane	45	415	80	28	27
CH_2DCH_2CN out-of-plane	58	496	74	29	28
CH_3CHDCN	55	222	71	29	57[b]
$CH_3CH_2C^{15}N$	67	270	78	31	64[b]

[a] Calculated from the median of absolute deviations; [b] for the millimeter wave transitions, the standard deviation of the microwave transitions is 16 kHz.

Table 2. Spectroscopic constants of the ground vibrational state of CH_3CHDCN, CH_2DCH_2CN and $CH_3CH_2C^{15}N$.

	CH_2DCH_2CN in-plane	CH_2DCH_2CN out-of-plane	CH_3CHDCN	$CH_3CH_2C^{15}N$
A /MHz	27651.28641(85)	25022.90806(62)	24449.0602(15)	27541.8853(13)
B /MHz	4425.144021(82)	4583.488572(88)	4661.39671(21)	4574.82824(19)
C /MHz	4000.798104(76)	4110.239468(83)	4155.45941(20)	4119.44781(19)
Δ_J /kHz	2.565394(33)	3.122672(31)	2.839982(82)	2.893555(79)
Δ_{JK} /kHz	–45.12388(92)	–39.91080(59)	-34.0809(14)	-46.1359(13)
Δ_K /kHz	551.5425(70)	405.8505(38)	365.720(24)	547.265(14)
δ_j /Hz	550.855(23)	703.046(20)	656.296(27)	635.249(38)
δ_k /kHz	10.8468(55)	11.0888(26)	11.6287(44)	12.5398(81)
Φ_J /mHz	7.5447(37)	9.9689(35)	8.4837(98)	8.9909(84)
Φ_{JK} /mHz	–54.29(79)	–34.13(73)	–	–20.9(11)
Φ_{KJ} /Hz	–1.3293(42)	–1.3663(31)	–1.1188(27)	–1.9066(62)
Φ_K /Hz	28.440(21)	18.8395(90)	15.57(10)	30.827(44)
ϕ_j /mHz	2.8196(28)	3.8411(23)	3.3694(40)	3.4096(49)
ϕ_{jk} /mHz	78.25(65)	101.06(39)	85.03(74)	103.26(85)
ϕ_k /Hz	5.618(63)	4.153(46)	4.067(12)	6.561(84)
L_{JK} /MHz	–	–	–	–6.45(27)
L_{KKJ} /MHz	38.7(27)	48.04(99)	–	101.5(24)
l_k /MHz	279.(14)	236.7(61)	317.(14)	–

Standard deviation of the fits are given Table 1, see text for more details. Uncertainties given in parenthesis are in units of the last digit given and 1 times the standard deviation.

standard least squares fitting methods and automatically rejecting most of the misassigned lines.

The number of measured lines, the maximum value of J and K_a, and the standard deviation of the fits are presented in Table 1 for the four studied species: $CH_3CH_2C^{15}N$, CH_2DCH_2CN in-plane, CH_2DCH_2CN out-of-plane, and CH_3CHDCN. For the $CH_3CH_2C^{15}N$ and CH_3CHDCN species, it is possible to reduce the standard deviation of the fit slightly by using higher order centrifugal distortion constants; but they are only marginally determined and they worsen the precision of the predictions. They were therefore no longer considered. The spectroscopic parameters derived from the fitting procedure are presented in Table 2. The list of measured lines are accessible in the online section as Tables 3–6 for $CH_3CH_2C^{15}N$, CH_3CHDCN, CH_2DCH_2CN in-plane, and CH_2DCH_2CN out-of-plane, respectively. For each measured line, the tables indicate its assignment (quantum numbers), the measured frequency, the difference between the observed and calculated frequency, the line strength, the dipole component, and the energy of the lower level.

The frequency range of the measurements (8–660 GHz) and the value of the quantum numbers of the identified lines ($J \leq 80$ and $K_a \leq 31$) are suitable for astronomical studies. Ethyl cyanide is present in hot cores and has a rather high temperature, in the 100–300 K range, as its isotopologues should also have. For such temperatures (100 and 300 K), the most intense rotational transitions of ethyl cyanide occur around 238 and 407 GHz, respectively, corresponding to J values of 25 and 45, respectively. The set of spectroscopic parameters derived for each species thus allows us to predict reliably the line frequencies and the band intensity of the transitions in the spectral range suitable for interstellar detection. For each species we have calculated a prediction of the rotational spectrum in the 8–1000 GHz range for $J \leq 80$ and $K_a \leq 31$. A short sample of the predictions is shown in the online section for each isotopologues (Tables 7–10), the entire tables are available in electronic form at the CDS. The tables indicate the quantum numbers of the transition, the calculated frequency and uncertainty, the line strength, the dipole component and the energy of the lower level. The calculated error (third column in the tables) is estimated from the accuracy of the spectroscopic parameters derived by the fitting procedure. However, to get a more realistic estimation of the error, it must be multiplied by a factor 3 for the strongest lines to 10, for the weakest lines. The precision on the line frequency is good enough for line identification in interstellar spectra. For the lines that are the most suitable for detection, i.e., the strongest lines having J value up to ∼50–60 and a low K_a value, the error on the predicted frequencies is a few hundred kHz. The error is larger for the weakest lines and increases as J and K_a become larger, i.e., as the frequency increases.

4. $CH_3CH_2C^{15}N$ detection in Orion

4.1. Astronomical observation

The observations were carried out using the IRAM 30 m radio telescope during 2004 September (3 mm and 1.3 mm), 2005 March (2 mm), 2005 April (3 mm and 1.3 mm). We acquired data for the entire spectral range detectable by the 30-m

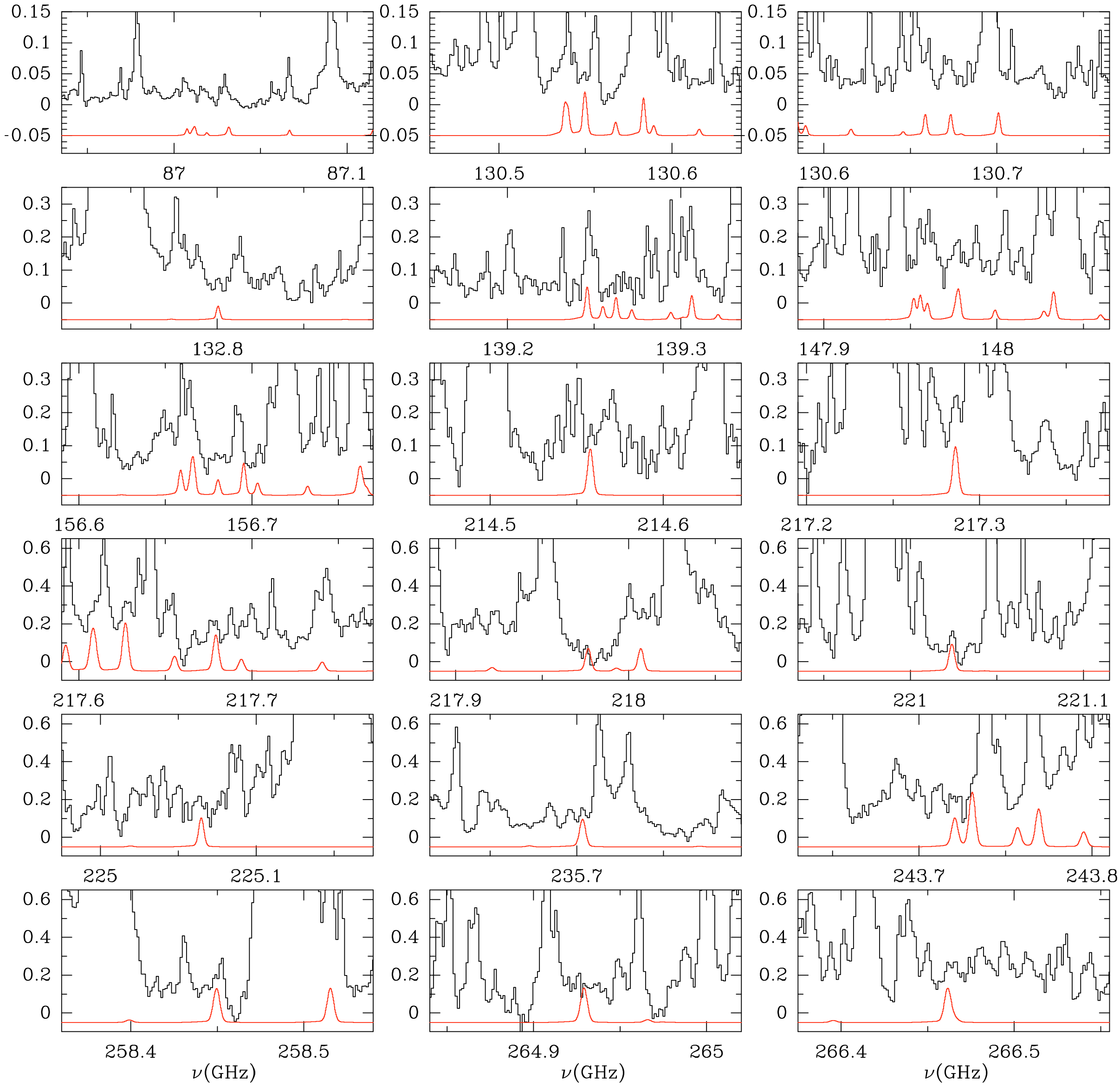

Fig. 1. ^{15}N-ethyl cyanide isotopologues detection in Orion. The spectra are in units of main beam temperature ($T_{\rm mb}$). The histogram spectra offset with respect to each other are the observations (black curve) and the model (smooth red line).

recievers. The four SiS receivers operating at 3, 2 and 1.3 mm were used simultaneously. Each receiver was tuned to a single sideband with image rejections within 20−27 dB (3 mm receivers), 12−16 dB (2 mm receivers), and 13 dB (1.3 mm receivers).

System temperatures were 100−350 K for the 3 mm receivers, 200−500 K for the 2 mm receivers, and 200−800 K for the 1.3 mm receivers, depending on the particular frequency, weather conditions, and source elevation. The intensity scale was calibrated using two absorbers at different temperatures and using the Atmospheric Transmission Model (Cernicharo 1985; Pardo et al. 2001).

Pointing and focus were regularly monitored by observing the nearby quasars 0420-014 and 0528+134. The observations were completed in the balanced wobbler-switching mode with a wobbling frequency of 0.5 Hz and a beam throw in azimuth of ±240″. The backends used were two filter banks with 512 × 1 MHz channels and a correlator providing two 512 MHz bandwidths and 1.25 MHz resolution. We performed a spectral-line survey, for which the central frequencies were chosen in a systematic way: from 80 GHz to 115.5 GHz for the 3 mm domain; from 130.25 GHz to 176.75 GHz for 2 mm; from 197 to 241 GHz for 1.3 mm (low frequency) and from 241.25 to 281.75 GHz for the 1.3 mm domain (high frequency), in steps of 500 MHz. We pointed toward the (survey) position α = $5^{\rm h}35^{\rm m}14.5^{\rm s}$, $\delta = -5°22'30.0''$ (J2000.0), corresponding to IRc2. The detailed procedure used for the analysis of the line survey is described in Tercero et al. (in preparation).

4.2. Astronomical modeling

In agreement with previous observations of Orion, four clearly defined kinematic regions with quite different physical and chemical conditions (Blake et al. 1987, 1996) are implied by the observed LSR velocities and line widths: (i) the narrow ($\lesssim$5 km s^{-1} line width) feature at $v_{\rm LSR} \simeq 9$ km s^{-1}, forming a N-S *extended ridge* or ambient cloud; (ii) a compact and quiescent region, *compact ridge*, ($v_{\rm LSR} \simeq 8$ km s^{-1}, $\Delta v \simeq 3$ km s^{-1}), identified for the first time by Johansson et al. (1984); (iii) the more turbulent and compact *plateau* ($v_{LSR} \simeq 6-10$ km s^{-1}, $\Delta v \gtrsim 25$ km s^{-1}); (iv) the *hot core* component ($v_{LSR} \simeq 3-5$ km s^{-1}, $\Delta v \lesssim 10-15$ km s^{-1}), first observed in ammonia emission (Morris et al. 1980).

In modeling the emission from the ^{15}N isotopologue of ethyl cyanide, we found that, as for the ^{13}C isotopologues (Demyk et al. 2007), a sum of two components is sufficient to reproduce all line intensities and profiles reasonably well: the hot core component and the plateau. We assumed LTE for both components. For the hot core, a column density of 3×10^{14} cm^{-2}, a line width of 5 km s^{-1}, and a rotational temperature of 300 K were the most suitable parameters for reproducing the bulk of the $CH_3CH_2C^{15}N$ emission. A broad velocity component is also required to reproduce the observations accurately, corresponding to the plateau for which we obtain a column density of 1×10^{13} cm^{-2}, a line width of 20 km s^{-1}, and a rotational temperature of 150 K. For the hot core component, we assumed a source diameter of 7″ with uniform brightness temperature and optical depth over its extent at 3″ from the pointed position (the observation were pointed towards IRc2, while the CN bearing species appears to originate in a small region 3″ North). For the plateau component, we assumed a size for the source of 30″.

The lines of $CH_3CH_2C^{15}N$ are weak and many of them are heavily blended with lines from other species. However, no missing lines were found in the coverage of our line survey of Orion and the lines of $CH_3CH_2C^{15}N$ free of blending appear at the correct frequencies and with the correct intensities. Although our modeling lacks a robust analysis, the difference between model and observed intensities is always below 20%. Our modeling of the different components is straightforward, although we emphasize that we modeled the main isotope, for which strong lines are observed, with the same model and the lines are well reproduced. Hence, we are confident about the results for the isotope ^{15}N, in particular that the frequency of all detected lines differ from laboratory measurements by less than 0.5 MHz. Hence, our assignment of the lines shown in Fig. 1 and in Table 11 to the ^{15}N isotopologue is fairly secure. The procedure that we used to identify the carriers of the weak lines in Orion, many of which remain unassigned at present, is the most suitable for this source since it permits to confirm whether there are no missing lines of the molecules for which we are looking.

Figure 1 shows selected observed lines of the ^{15}N isotopologue with model results. Table 11 (see online material) indicates the model predictions, observed peak intensities and frequencies, and predicted frequencies from the rotational constants obtained in this paper, for all lines of $CH_3CH_2C^{15}N$ that were not strongly blended with other lines. The differences between the intensity of the model and the peak intensity of the observed lines were mostly due to the contribution from many other molecular species (the strong overlap with other lines ensures that it is difficult to provide a good baseline for the weak lines of $CH_3CH_2C^{15}N$).

Using the column density derived for the ^{13}C isotopologues (1.6×10^{15} and 6×10^{13} cm^{-2} for the hot core and the plateau, respectively; see Demyk et al. 2007), we derive an isotopic ratio ^{13}C/^{15}N of between 5−6, in agreement with the solar isotopic abundance (^{13}C/^{15}N (solar) $\simeq 6$) and strengthening our identification of ^{15}N-ethyl cyanide in Orion. The detailed modeling of ethyl cyanide including the main isotopologue, the vibrationally excited states and the detected isotopologues, will be published elsewhere (Tercero et al., in preparation).

Deuterated ethyl cyanide has not been detected in this line survey above the line confusion limit. Assuming the same physical conditions as those derived for $CH_3CH_2C^{15}N$, we have derived an upper limit to the column densities of CH_2DCH_2CN (in-plane and out-of-plane) of 1×10^{14} cm^{-2} in both species.

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Table 3. Measured transitions of the ground vibrational state of $CH_3CH_2C^{15}N$.

Transition						Obs. Freq. (MHz)	obs.- calc. (MHz)	S	Dipole	E_l (cm^{-1})
J'	K'_a	K'_c	J''	K''_a	K''_c					
13	2	11	13	2	12	8439.616	0.003	5.5270	a	29.44
27	6	22	28	5	23	8579.609	–0.004	4.3669	b	137.32
1	0	1	0	0	0	8694.274	0.010	1.0000	a	0.00
27	6	21	28	5	24	8864.577	0.008	4.3657	b	137.31
31	4	27	31	4	28	9029.287	–0.011	0.8976	a	156.65
30	5	26	29	6	23	9223.293	–0.017	4.7882	b	154.18
61	7	54	61	7	55	9230.917	–0.004	1.3312	a	587.92
7	2	5	8	1	8	9270.407	0.020	1.0280	b	10.93
22	3	19	22	3	20	9468.661	–0.003	0.7197	a	80.47
6	1	5	6	1	6	9554.530	0.005	0.3102	a	6.70
41	5	36	41	5	37	9774.927	–0.010	1.0376	a	269.87
30	5	25	29	6	24	9780.015	–0.010	4.7908	b	154.17
51	6	45	51	6	46	9786.557	0.007	1.1824	a	413.66
15	2	14	14	3	11	9904.529	–0.014	2.2952	b	37.48
46	8	39	45	9	36	10 289.690	0.000	7.3345	b	363.08
46	8	38	45	9	37	10 303.589	–0.022	7.3346	b	363.08
14	2	12	14	2	13	10 999.282	0.002	0.5055	a	33.48
62	7	55	62	7	56	11 195.294	–0.016	1.2899	a	605.99
25	4	22	24	5	19	11 277.619	0.002	4.0009	b	106.47
32	4	28	32	4	29	11 288.624	–0.010	0.8540	a	165.97
32	7	26	33	6	27	11296.821	0.000	5.1435	b	190.82
32	7	25	33	6	28	11 373.145	0.036	5.1432	b	190.82
16	4	13	17	3	14	11 475.918	0.001	2.6021	b	51.48
12	1	12	11	2	9	11 634.396	–0.012	1.2301	b	22.36
52	6	46	52	6	47	11 946.306	0.015	1.1406	a	428.82
23	3	20	23	3	21	11 978.970	–0.011	0.6755	a	87.15
42	5	37	42	5	38	12 042.892	–0.022	0.9951	a	282.11
20	3	18	19	4	15	12 079.320	0.008	3.1893	b	67.57
5	2	4	6	1	5	12 719.608	0.008	0.9101	b	7.02
7	1	6	7	1	7	12 732.353	0.003	0.2689	a	8.68
4	0	4	3	1	3	12 851.255	0.004	1.6107	b	2.47
41	7	35	40	8	32	13 094.510	–0.015	6.5569	b	287.57
11	3	8	12	2	11	13 420.087	0.028	1.7745	b	25.68
63	7	56	63	7	57	13 500.281	0.023	1.2487	a	624.34
14	2	12	13	3	11	13 834.054	0.009	2.3230	b	33.39
33	4	29	33	4	30	13 961.689	–0.009	0.8118	a	175.57
37	8	30	38	7	31	13 970.932	–0.011	5.9196	b	253.11
37	8	29	38	7	32	13 990.537	0.003	5.9195	b	253.11
15	2	13	15	2	14	14 012.666	–0.001	0.4639	a	37.81
53	6	47	53	6	48	14 483.258	–0.006	1.0990	a	444.27
43	5	38	43	5	39	14 713.143	–0.014	0.9534	a	294.64
21	5	17	22	4	18	14 851.715	–0.007	3.3752	b	85.92
24	3	21	24	3	22	14 935.533	–0.007	0.6340	a	94.12
13	1	13	12	2	10	15 425.057	–0.014	1.2023	b	25.89
21	5	16	22	4	19	15 563.277	0.004	3.3716	b	85.89
6	2	4	7	1	7	15 696.387	0.017	0.8951	b	8.68
36	6	31	35	7	28	15 803.117	0.011	5.7777	b	220.84
36	6	30	35	7	29	16 013.770	0.026	5.7786	b	220.84
64	7	57	64	7	58	16 186.292	0.012	1.2076	a	642.99
8	1	7	8	1	8	16 356.925	–0.004	0.2377	a	10.93
52	9	44	51	10	41	16 396.371	–0.013	8.3221	b	462.17
42	9	34	43	8	35	16 671.014	–0.002	6.6953	b	324.19
10	3	8	11	2	9	16 882.196	0.004	1.6202	b	22.36
2	1	2	1	1	1	16 933.357	0.023	1.5000	a	1.06
34	4	30	34	4	31	17 086.864	0.039	0.7710	a	185.47
16	2	15	15	3	12	17 185.449	–0.005	2.4300	b	41.85
2	0	2	1	0	1	17 381.760	0.002	0.4273	a	42.42
16	2	14	16	2	15	17 495.223	0.009	1.9999	a	0.29
2	1	1	1	1	0	17 843.970	0.016	1.5000	a	1.07
1	1	0	1	0	1	23 422.150	0.195	1.5000	b	0.29
2	1	1	2	0	2	23 884.160	0.009	2.4753	b	0.87
3	1	2	3	0	3	24 589.950	0.017	3.4137	b	1.74
3	1	3	2	1	2	25 395.730	0.020	2.666	a	1.62
3	0	3	2	0	2	26 055.770	0.050	2.9994	a	0.87

Table 3. continued.

Transition						Obs. Freq.	obs.- calc.	S	Dipole	E_l
J'	K'_a	K'_c	J''	K''_a	K''_c	(MHz)	(MHz)			(cm^{-1})
3	2	2	2	2	1	26 083.700	0.077	1.6667	a	3.96
3	2	1	2	2	0	26 110.300	–0.118	1.6667	a	3.96
3	1	2	2	1	1	26 761.440	–0.062	2.6666	a	1.67
1	1	1	0	0	0	31 660.920	0.026	2.6666	b	0.00
2	1	2	1	0	1	39 899.960	–0.004	1.5000	b	0.29
20	1	20	19	1	19	167 736.896	0.066	1.5000	a	54.16
20	0	20	19	0	19	168 308.099	0.086	19.9316	a	54.05
20	2	19	19	2	18	172 402.970	0.120	19.9403	a	57.98
20	8	13	19	8	12	174 074.577	0.088	19.7808	a	104.59
20	9	12	19	9	11	174 075.603	0.101	16.8004	a	117.71
20	10	11	19	10	10	174 088.863	0.086	15.9504	a	132.35
20	7	14	19	7	13	174 091.333	0.102	15.0004	a	93.02
20	11	9	19	11	8	174 111.289	0.044	17.5504	a	148.52
20	6	14	19	6	13	174 136.505	0.003	13.9503	a	82.98
20	6	15	19	6	14	174 136.505	0.094	18.2003	a	82.98
20	12	9	19	12	8	174 141.113	0.035	18.2003	a	166.22
20	13	7	19	13	6	174 177.165	0.041	12.8003	a	185.43
20	14	6	19	14	5	174 218.677	0.051	11.5503	a	206.16
20	5	16	19	5	15	174 231.742	0.016	10.2002	a	74.50
20	5	15	19	5	14	174 235.852	0.023	18.7502	a	74.50
20	15	6	19	15	5	174 265.094	0.029	18.7502	a	228.39
20	3	18	19	3	17	174 273.451	0.100	8.7502	a	62.16
20	16	4	19	16	3	174 316.107	0.033	19.5460	a	252.13
20	17	3	19	17	2	174 371.426	0.042	7.2002	a	277.36
20	4	17	19	4	16	174 391.672	0.068	5.5501	a	67.56
20	19	1	19	19	0	174 494.185	0.048	19.1996	a	332.27
20	4	16	19	4	15	174 501.063	0.113	1.9500	a	67.57
20	3	17	19	3	16	175 670.653	0.064	19.1996	a	62.30
21	0	21	20	0	20	176 494.285	0.054	19.5487	a	59.67
20	2	18	19	2	17	177 778.527	0.026	20.9391	a	59.00
22	0	22	21	0	21	184 683.451	0.089	19.8087	a	65.55
21	3	18	20	3	17	184 690.770	0.072	21.9381	a	68.16
23	1	23	22	1	22	192 539.029	0.046	20.5706	a	71.78
23	0	23	22	0	22	192 876.014	0.075	22.9334	a	71.71
18	2	17	17	1	16	193 737.725	–0.040	22.9373	b	46.05
22	3	19	21	3	18	193 741.168	–0.069	7.2189	a	74.32
37	3	35	37	2	36	193 807.027	–0.155	21.5910	b	204.24
23	1	23	22	0	22	194 359.838	0.062	14.1553	b	71.71
9	3	6	8	2	7	194 740.388	0.127	18.9865	b	13.53
23	2	22	22	2	21	197 751.274	0.129	3.4828	a	76.07
23	9	15	22	9	14	200 193.855	0.113	22.7981	a	136.00
23	10	14	22	10	13	200 201.229	0.082	19.4787	a	150.64
23	8	16	22	8	15	200 203.741	0.098	18.6526	a	122.88
23	11	13	22	11	12	200 221.198	0.007	20.2178	a	166.82
23	7	17	22	7	16	200 239.243	0.015	17.7396	a	111.31
23	12	12	22	12	11	200 251.135	0.036	20.8700	a	184.52
23	13	10	22	13	9	200 289.205	0.076	16.7395	a	203.73
23	3	21	22	3	20	200 307.620	0.082	15.6525	a	80.47
23	14	9	22	14	8	200 334.120	–0.015	22.6012	a	224.47
23	15	9	22	15	8	200 385.331	–0.008	14.4786	a	246.70
23	1	22	22	1	21	200 425.298	0.050	13.2177	a	75.29
23	16	7	22	16	6	200 442.189	–0.002	22.8741	a	270.44
23	5	19	22	5	18	200 466.463	0.129	11.8698	a	92.81
23	5	18	22	5	17	200 480.816	0.035	21.9131	a	92.81
23	17	6	22	17	5	200 504.312	0.022	21.9131	a	295.68
23	18	5	22	18	4	200 571.389	0.053	10.4350	a	322.40
23	19	4	22	19	3	200 643.145	0.046	8.9133	a	350.60
23	4	20	22	4	19	200 669.063	0.120	7.3045	a	85.89
29	5	24	29	4	25	200 693.272	–0.036	22.3034	b	139.07
23	20	3	22	20	2	200 719.345	–0.051	16.0583	a	380.28
24	1	24	23	1	23	200 793.296	0.102	5.6088	a	78.20
23	21	2	22	21	1	200 800.105	0.026	23.9337	a	411.42
23	22	1	22	22	0	200 885.025	–0.001	3.8262	a	444.03
23	4	19	22	4	18	200 952.117	0.023	1.9566	a	85.92
28	5	23	28	4	24	202 003.528	–0.075	22.3036	b	130.58

Table 3. continued.

Transition						Obs. Freq.	obs.- calc.	S	Dipole	E_l
J'	K'_a	K'_c	J''	K''_a	K''_c	(MHz)	(MHz)			(cm^{-1})
24	1	24	23	0	23	202 277.181	0.150	15.3800	b	78.15
23	3	20	22	3	19	202 817.910	0.055	20.0098	a	80.79
27	5	22	27	4	23	203 124.417	–0.017	22.6101	b	122.39
26	5	21	26	4	22	204 076.918	–0.055	14.7154	b	114.50
23	2	21	22	2	20	204 419.505	0.010	14.0626	a	77.68
25	5	20	25	4	21	204 881.818	0.014	22.8303	b	106.91
24	5	19	24	4	20	205 558.318	0.022	13.4202	b	99.62
31	5	27	31	4	28	205 711.989	–0.056	12.7872	b	156.65
32	5	28	32	4	29	205 713.735	0.039	17.2162	b	165.97
30	5	26	30	4	27	205 774.851	–0.004	17.8631	b	147.62
33	5	29	33	4	30	205 793.562	–0.068	16.5700	b	175.57
29	5	25	29	4	26	205 889.044	–0.077	18.5090	b	138.88
34	5	30	34	4	31	205 966.280	–0.025	15.9257	b	185.47
23	5	19	23	4	20	207 061.424	0.037	19.1522	b	92.59
22	5	18	22	4	19	207 264.077	0.082	12.1465	b	85.89
20	5	15	20	4	16	207 308.973	–0.035	11.5344	b	73.39
21	5	17	21	4	18	207 454.740	–0.039	10.3294	b	79.49
36	4	33	36	2	34	207 629.152	–0.065	10.9273	a	199.21
20	5	16	20	4	17	207 630.890	–0.121	0.1443	b	73.38
38	5	34	38	4	35	207 884.134	–0.016	10.3249	b	227.95
18	5	14	18	4	15	207 933.343	–0.077	21.6546	b	62.04
17	5	12	17	4	13	207 966.998	0.145	9.1323	b	56.81
17	5	13	17	4	14	208 058.204	–0.094	8.5419	b	56.81
16	5	11	16	4	12	208 108.794	0.004	8.5409	b	51.87
27	1	27	26	1	26	225 525.534	0.024	7.9523	a	99.12
27	0	27	26	0	26	225 679.061	0.088	26.9341	a	99.09
48	5	44	48	4	45	225 893.897	–0.039	26.9355	b	354.12
45	6	39	45	5	40	228 751.245	0.064	26.5948	b	321.29
49	5	45	49	4	46	228 977.623	0.001	26.6357	b	368.28
43	6	37	43	5	38	234 586.186	0.030	26.9371	b	295.13
27	3	25	26	3	24	234 807.785	–0.021	24.9776	a	108.93
27	10	18	26	10	17	235 016.788	0.026	26.6513	a	179.10
27	9	19	26	9	18	235 022.338	0.008	23.2969	a	164.45
27	11	17	26	11	16	235 029.774	–0.019	24.0006	a	195.28
27	8	20	26	8	19	235 054.039	–0.028	22.5191	a	151.34
27	12	15	26	12	14	235 056.914	–0.022	24.6302	a	212.98
27	13	14	26	13	13	235 095.448	0.066	21.6672	a	232.20
27	7	21	26	7	20	235 125.658	0.037	20.7412	a	139.77
27	14	14	26	14	13	235 143.241	–0.052	25.1857	a	252.94
27	15	12	26	15	11	235 199.461	0.040	19.7412	a	275.18
27	6	22	26	6	21	235 262.890	–0.106	18.6671	a	298.93
27	16	11	26	16	10	235 262.890	0.002	17.5189	a	129.76
27	6	21	26	6	20	235 265.575	0.038	25.6670	a	129.76
27	17	10	26	17	9	235 333.048	–0.013	25.6670	a	324.17
27	18	10	26	18	9	235 409.551	0.085	16.2967	a	350.90
27	19	8	26	19	7	235 491.756	0.010	15.0004	a	379.12
27	5	23	26	5	22	235 502.449	0.137	13.6299	a	121.31
27	5	22	26	5	21	235 562.287	–0.021	26.0740	a	121.31
27	20	7	26	20	6	235 579.580	–0.038	26.0740	a	408.81
27	21	7	26	21	6	235 672.776	–0.081	12.1855	a	439.96
27	4	24	26	4	23	235 703.253	0.085	10.6669	a	114.42
27	22	6	26	22	5	235 771.204	–0.076	26.4051	a	472.57
27	23	5	26	23	4	235 874.643	–0.089	9.0743	a	506.64
27	24	4	26	24	3	235 983.039	–0.042	7.4076	a	542.15
27	25	2	26	25	1	236 096.141	–0.073	5.6668	a	579.08
27	26	1	26	26	0	236 213.988	–0.040	3.8519	a	617.45
27	4	23	26	4	22	236 514.897	0.050	1.9630	a	114.50
42	6	36	42	5	37	237 090.840	–0.040	26.4061	b	282.51
27	3	24	26	3	23	239 246.369	0.185	24.1944	a	109.67
27	2	25	26	2	24	239 319.446	–0.060	26.6778	a	106.71
68	4	65	67	4	64	580 855.280	–0.026	26.8350	a	670.35
68	3	65	67	3	64	581 096.046	0.009	67.6014	a	670.31
38	6	32	37	5	33	581 630.984	–0.133	67.6028	b	223.81
27	8	20	26	7	19	581 840.825	–0.066	10.4679	b	139.77
67	12	56	66	12	55	582 271.259	0.042	10.5477	a	752.66
68	4	65	67	3	64	582 281.145	–0.226	64.8540	b	670.31

Table 3. continued.

Transition						Obs. Freq.	obs.- calc.	S	Dipole	E_l
J'	K'_a	K'_c	J''	K''_a	K''_c	(MHz)	(MHz)			(cm^{-1})
69	3	67	68	2	66	582 523.118	–0.055	40.2247	b	677.75
67	21	47	66	21	46	582 538.739	0.066	49.7614	a	980.48
70	1	69	69	1	68	584 132.577	–0.266	60.4197	a	683.93
70	2	69	69	2	68	584 132.577	0.126	69.8085	a	683.93
69	4	65	68	5	64	585 001.536	0.077	69.8085	b	700.58
67	7	61	66	7	60	585 031.259	0.092	31.4924	a	681.15
71	0	71	70	0	70	585 864.038	–0.103	66.2636	a	689.02
33	7	27	32	6	26	586 609.713	–0.132	70.9336	b	181.22
33	7	26	32	6	27	586 664.531	–0.089	10.8318	b	181.22
68	5	64	67	5	63	587 123.079	0.024	10.8314	a	681.00
69	3	66	68	4	65	588 007.013	0.012	67.5186	b	689.73
69	4	66	68	4	65	588 990.953	0.011	41.2613	a	689.73
68	4	64	67	4	63	589 093.108	0.019	68.6004	a	680.53
67	7	60	66	7	59	589 103.047	0.012	67.5370	a	681.91
12	11	1	11	10	2	589 148.105	0.029	66.2850	b	96.35
69	3	66	68	3	65	589 192.334	–0.001	10.5262	a	689.69
28	8	20	27	7	21	590 484.158	–0.171	68.6016	b	147.62
28	8	21	27	7	20	590 484.158	0.006	10.7341	b	147.62
67	5	62	66	5	61	590 550.631	0.114	10.7341	a	668.66
68	16	53	67	16	52	590 583.268	0.109	66.5724	a	858.12
70	3	68	69	3	67	590 586.082	–0.015	64.2378	a	697.18
70	2	68	69	2	67	590 596.898	–0.021	69.6965	a	697.18
68	14	55	67	14	54	590 617.504	0.100	69.6965	a	812.00
68	17	51	67	17	50	590 634.699	0.027	65.1206	a	883.47
68	18	50	67	18	49	590 721.807	0.095	63.7524	a	910.34
68	13	56	67	13	55	590 726.943	0.083	63.2375	a	791.26
68	19	50	67	19	49	590 839.222	0.086	65.5178	a	938.71
68	12	56	67	12	55	590 923.453	0.076	62.6933	a	772.08
68	20	48	67	20	47	590 983.062	–0.007	65.8857	a	968.57
68	21	48	67	21	47	591 150.609	0.074	62.1196	a	999.91
68	22	47	67	22	46	591 339.235	0.023	61.5166	a	1032.73
68	23	45	67	23	44	591 547.296	0.046	60.8841	a	1067.02
68	10	59	67	10	58	591 726.616	0.057	60.2222	a	738.52
68	10	58	67	10	57	591 734.279	0.042	66.5335	a	738.52
68	24	44	67	24	43	591 773.206	0.043	66.5335	a	1102.76
68	6	63	67	6	62	591 820.411	0.036	59.5310	a	690.80
68	25	43	67	25	42	592 015.740	0.008	67.4236	a	1139.95
71	1	70	70	1	69	592 269.872	–0.215	58.8103	a	703.42
71	2	70	70	2	69	592 269.872	0.097	70.8084	a	703.42
68	26	43	67	26	42	592 273.970	0.024	70.8084	a	1178.57
68	9	60	67	9	59	592 451.332	0.036	58.0602	a	724.21
68	9	59	67	9	58	592 546.852	0.071	66.8133	a	724.22
68	28	41	67	28	40	592 834.062	0.022	66.8134	a	1260.10
68	29	40	67	29	39	593 134.581	0.007	56.4718	a	1302.98
23	9	15	22	8	14	593 302.090	–0.058	55.6334	b	122.88
68	30	38	67	30	37	593 448.046	0.029	10.5229	a	1347.25
68	7	62	67	7	61	593 678.914	0.040	54.7657	a	700.66
68	31	37	67	31	36	593 773.970	0.079	67.2729	a	1392.92
68	32	37	67	32	36	594 111.791	0.020	53.8686	a	1439.96
68	8	60	67	8	59	594 207.496	0.016	52.9420	a	711.74
68	33	36	67	33	35	594 461.221	–0.053	67.0645	a	1488.37
34	7	28	33	6	27	595 059.426	–0.114	51.9861	b	190.82
34	7	27	33	6	28	595 138.148	–0.045	10.9923	b	190.82
18	10	9	17	9	8	595 699.942	–0.004	10.9917	b	106.96
70	3	67	69	4	66	596 306.359	–0.001	10.3865	b	709.38
70	4	67	69	4	66	597 122.122	0.008	42.3040	a	709.38
70	3	67	69	3	66	597 290.338	0.038	69.5995	a	709.34
13	11	2	12	10	3	597 873.058	0.047	69.6005	b	99.83
68	7	61	67	7	60	598 287.464	–0.015	10.5889	a	701.56
41	6	36	40	5	35	598 616.486	–0.140	67.2997	b	258.18
68	5	63	67	5	62	598 643.423	0.015	10.8027	a	688.36
71	2	69	70	3	68	598 679.183	–0.041	67.5609	b	716.88
71	3	69	70	3	68	598 716.775	–0.074	51.7788	a	716.88
71	2	69	70	2	68	598 725.617	–0.030	70.6961	a	716.88

Table 3. continued.

Transition						Obs. Freq.	obs.- calc.	S	Dipole	E_l
J'	K'_a	K'_c	J''	K''_a	K''_c	(MHz)	(MHz)			(cm^{-1})
29	8	22	28	7	21	599 117.241	0.059	70.6961	b	155.75
73	1	73	72	1	72	602 139.639	–0.062	10.9191	a	728.38
73	2	72	72	2	71	608 536.328	0.068	72.9336	a	743.20
73	3	71	72	3	70	614 970.125	–0.012	72.8083	a	757.09
37	7	31	36	6	30	620 201.609	–0.128	72.6954	b	221.38
14	14	0	14	13	1	621 173.893	0.035	11.4503	b	160.74
16	14	3	16	13	4	621 242.739	0.010	0.9765	b	169.75
17	14	3	17	13	4	621 279.788	0.044	2.7597	b	174.69
19	14	6	19	13	7	621 358.456	–0.007	3.5863	b	185.43
20	14	6	20	13	7	621 399.807	–0.158	5.1434	b	191.24
21	14	8	21	13	9	621 442.763	0.012	5.8837	b	197.34
22	14	9	22	13	10	621 486.697	–0.010	6.6033	b	203.73
73	4	70	72	4	69	621 491.509	0.024	7.3053	a	769.94
23	14	10	23	13	11	621 531.689	–0.025	72.5970	b	210.42
73	3	70	72	3	69	621 588.534	0.019	7.9920	a	769.92
25	14	12	25	13	13	621 624.366	–0.009	72.5975	b	224.65
26	14	12	26	13	13	621 671.747	–0.017	9.3274	b	232.20
28	14	14	28	13	15	621 767.960	–0.003	9.9793	b	248.17
29	14	16	29	13	17	621 816.544	0.066	11.2575	b	256.60
21	10	12	20	9	11	621 856.005	–0.034	11.8860	b	123.51
30	14	16	30	13	17	621 864.978	–0.087	10.8992	b	265.31
76	0	76	75	0	75	626 532.225	–0.020	12.5085	a	789.45
73	5	69	72	5	68	627 977.934	0.042	75.9337	a	781.65
27	9	19	26	8	18	628 061.087	–0.080	72.5136	b	151.34
73	4	69	72	4	68	628 944.325	0.044	11.2781	a	781.44
22	10	13	21	9	12	630 571.790	–0.029	72.5207	b	129.61
17	11	7	16	10	6	632 779.134	–0.001	11.0782	b	116.67
76	2	75	75	2	74	632 915.087	0.035	11.0394	a	804.91
33	8	25	32	7	26	633 529.416	–0.124	75.8082	b	191.20
73	6	68	72	6	67	633 537.393	0.015	11.6419	a	792.30
73	16	58	72	16	57	633 629.268	–0.017	72.4319	a	959.49
73	15	59	72	15	58	633 647.418	0.021	69.4962	a	935.67
73	17	57	72	17	56	633 661.718	–0.007	69.9211	a	984.85
73	14	60	72	14	59	633 728.218	–0.005	69.0440	a	913.38
73	18	56	72	18	55	633 736.018	–0.021	70.3186	a	1011.73
73	19	54	72	19	53	633 845.800	–0.069	68.5643	a	1040.12
73	13	61	72	13	60	633 889.390	0.010	68.0573	a	892.66
73	20	54	72	20	53	633 986.396	–0.047	70.6888	a	1070.00
73	21	53	72	21	52	634 154.055	–0.055	67.5229	a	1101.38
73	12	61	72	12	60	634 157.490	–0.061	66.9611	a	873.52
73	12	62	72	12	61	634 157.490	0.051	71.0317	a	873.52
73	22	52	72	22	51	634 345.936	–0.091	71.0317	a	1134.23
73	23	51	72	23	50	634 559.857	–0.081	66.3719	a	1168.55
73	11	63	72	11	62	634 574.131	–0.040	65.7553	a	855.99
73	11	62	72	11	61	634 576.098	0.000	71.3472	a	855.99
77	0	77	76	0	76	634 657.408	0.002	71.3472	a	810.35
12	12	1	11	11	0	634 790.497	0.059	76.9337	b	112.52
73	24	50	72	24	49	634 793.917	–0.117	11.4949	a	1204.33
73	25	49	72	25	48	635 046.756	–0.080	65.1114	a	1241.56
73	10	64	72	10	63	635 203.088	–0.031	64.4400	a	840.11
73	10	63	72	10	62	635 229.566	–0.074	71.6355	a	840.11
73	26	48	72	26	47	635 317.043	–0.078	71.6355	a	1280.23
73	27	47	72	27	46	635 603.756	–0.109	63.7412	a	1320.33
73	28	46	72	28	45	635 906.292	0.092	63.0151	a	1361.85
73	9	65	72	9	64	636 091.034	–0.059	62.2616	a	825.94
73	29	45	72	29	44	636 223.427	0.047	71.8962	a	1404.78
73	30	44	72	30	43	636 554.706	–0.050	61.4806	a	1449.11
73	31	43	72	31	42	636 899.833	0.073	60.6723	a	1494.83
73	8	66	72	8	65	636 965.312	–0.056	59.8366	a	813.49
73	32	42	72	32	41	637 257.939	0.052	72.1263	a	1541.92
73	33	41	72	33	40	637 628.504	–0.182	58.9735	a	1590.39
73	5	68	72	5	67	638 398.590	–0.039	72.5031	a	790.87
73	8	65	72	8	64	638 971.382	–0.140	72.5031	a	813.83
76	3	74	75	3	73	639 329.193	0.009	72.1331	a	819.44
76	2	74	75	2	73	639 332.291	0.015	75.6945	a	819.44
77	1	76	76	1	75	641 035.637	–0.033	75.6946	a	826.02

Table 3. continued.

Transition						Obs. Freq.	obs.- calc.	S	Dipole	E_l
J'	K_a'	K_c'	J''	K_a''	K_c''	(MHz)	(MHz)			(cm^{-1})
78	0	78	77	0	77	642 779.680	0.014	76.8081	a	831.52
13	12	2	12	11	1	643 519.782	0.054	77.9337	b	116.00
73	7	66	72	7	65	644 245.408	–0.216	11.5231	a	804.41
29	9	20	28	8	21	645 406.965	–0.115	72.3782	b	167.31
73	6	67	72	6	66	645 763.670	–0.166	11.6560	a	797.73
76	4	73	75	4	72	645 828.535	0.014	72.5483	a	832.95
76	3	73	75	3	72	645 883.850	0.025	75.5947	a	832.94
77	2	75	76	2	74	647 445.714	0.024	75.5950	a	840.77
51	6	46	50	5	45	647 492.660	–0.021	76.6943	b	392.06
24	10	14	23	9	15	647 996.890	–0.115	11.5988	b	142.68
52	6	47	51	5	46	650 096.789	–0.055	11.4443	b	407.13
79	0	79	78	0	78	650 899.023	0.033	11.7312	a	852.96

Table 4. Measured transitions of the ground vibrational state of CH_3CHDCN.

Transition						Obs. Freq.	obs.- calc.	S	Dipole	E_l
J'	K'_a	K'_c	J''	K''_a	K''_c	(MHz)	(MHz)			(cm^{-1})
21	4	17	20	5	16	8145.638	–0.015	3.1333	b	78.57
36	5	31	36	5	32	8324.713	–0.032	1.1806	a	213.36
63	8	55	63	8	56	8399.871	–0.011	1.6500	a	637.87
7	1	6	6	2	5	8464.923	0.012	1.2346	b	8.85
9	3	7	10	2	8	8618.098	–0.003	1.3927	b	18.98
12	2	10	12	2	11	8717.220	0.009	0.5901	a	25.56
54	7	47	54	7	48	8805.418	–0.005	1.4898	a	471.24
45	6	39	45	6	40	8810.297	–0.001	1.3333	a	329.72
1	0	1	0	0	0	8816.849	0.004	1.0000	a	0.00
28	4	24	28	4	25	9391.902	0.008	0.9768	a	130.52
20	3	17	20	3	18	9748.892	0.009	0.7783	a	67.91
17	3	15	16	4	12	10 281.507	–0.001	2.5468	b	50.76
64	8	56	64	8	57	10 379.536	0.018	1.5968	a	656.81
10	1	10	9	2	7	10 485.947	–0.061	1.0465	b	16.00
37	5	32	37	5	33	10 561.366	–0.047	1.1258	a	224.31
6	1	5	6	1	6	10 611.891	–0.005	0.3106	a	6.66
18	5	14	19	4	15	10 639.881	0.001	2.7029	b	66.71
13	2	12	12	3	9	10 806.862	0.021	1.8927	b	29.01
27	7	21	28	6	22	10 903.039	0.026	4.0288	b	143.70
55	7	48	55	7	49	10 947.340	–0.003	1.4362	a	487.53
36	9	28	37	8	29	11 002.482	0.008	5.3534	b	249.85
46	6	40	46	6	41	11 044.227	–0.011	1.2791	a	343.34
18	5	13	19	4	16	11 169.908	–0.006	2.7004	b	66.69
13	2	11	13	2	12	11 552.330	0.006	0.5347	a	29.37
44	9	36	43	10	33	11 676.935	–0.018	6.5527	b	345.34
44	9	35	43	10	34	11 679.041	–0.001	6.5527	b	345.34
26	5	22	25	6	19	11 921.651	0.003	3.9003	b	119.79
35	7	29	34	8	26	11 931.913	–0.034	5.2284	b	218.00
35	7	28	34	8	27	11 963.341	–0.017	5.2285	b	218.00
29	4	25	29	4	26	11 977.187	0.006	0.9222	a	139.09
12	2	10	11	3	9	12 074.616	0.016	1.8603	b	25.45
4	2	3	5	1	4	12 302.830	0.025	0.6552	b	5.20
26	5	21	25	6	20	12 334.823	0.014	3.9022	b	119.79
21	3	18	21	3	19	12 565.691	0.025	0.7243	a	74.10
65	8	57	65	8	58	12 743.456	0.007	1.5435	a	676.05
5	2	3	6	1	6	12 975.003	0.037	0.7065	b	6.66
9	3	6	10	2	9	13 227.370	–0.001	1.3462	b	18.83
38	5	33	38	5	34	13 254.293	–0.018	1.0719	a	235.56
56	7	49	56	7	50	13 508.650	0.026	1.3825	a	504.11
47	6	41	47	6	42	13 722.075	–0.003	1.2254	a	357.26
7	1	6	7	1	7	14 137.108	–0.010	0.2697	a	8.66
17	3	14	16	4	13	14 455.726	0.068	2.5842	b	50.76
13	4	10	14	3	11	14 790.253	–0.001	1.9317	b	37.00
11	1	11	10	2	8	14 861.318	–0.028	1.0401	b	18.98
14	2	12	14	2	13	14 906.976	0.028	0.4868	a	33.46
30	4	26	30	4	27	15 067.432	–0.014	0.8696	a	147.96
31	8	24	32	7	25	15 504.979	0.018	4.5828	b	188.30
22	6	16	23	5	19	15 548.329	–0.025	3.2567	b	98.04
22	3	19	22	3	20	15 908.973	0.009	0.6740	a	80.58
13	4	9	14	3	12	16 164.630	–0.002	1.9235	b	36.95
39	5	34	39	5	35	16 455.692	–0.031	1.0191	a	247.10
57	7	50	57	7	51	16 543.426	0.014	1.3289	a	520.99
4	0	4	3	1	3	16 606.167	0.011	1.6423	b	2.38
48	6	42	48	6	43	16 897.855	0.023	1.1721	a	371.47
2	1	2	1	1	1	17 127.899	0.011	1.5000	a	0.95
19	1	19	18	1	18	160 885.388	0.018	18.9238	a	49.22
19	0	19	18	0	18	161 315.310	0.053	18.9303	a	49.15
19	2	18	18	2	17	165 755.106	0.042	18.7629	a	52.72
19	10	10	18	10	9	167 711.801	0.062	13.7374	a	117.07
19	9	11	18	9	10	167 713.718	0.069	14.7374	a	104.40
19	11	8	18	11	7	167 719.287	0.056	12.6321	a	131.05
19	8	12	18	8	11	167 728.769	0.047	15.6322	a	93.07
19	12	7	18	12	6	167 733.922	0.031	11.4215	a	146.36

Table 4. continued.

Transition						Obs. Freq.	obs.- calc.	S	Dipole	E_l
J'	K'_a	K'_c	J''	K''_a	K''_c	(MHz)	(MHz)			(cm^{-1})
19	13	7	18	13	6	167 754.360	0.042	10.1057	a	162.98
19	7	13	18	7	12	167 763.740	0.038	16.4216	a	83.06
19	14	5	18	14	4	167 779.610	0.016	8.6846	a	180.92
19	15	5	18	15	4	167 809.167	0.068	7.1582	a	200.17
19	6	14	18	6	13	167 831.864	0.155	17.1058	a	74.40
19	6	13	18	6	12	167 831.864	–0.044	17.1058	a	74.40
19	16	4	18	16	3	167 842.461	0.067	5.5265	a	220.72
19	17	2	18	17	1	167 879.190	0.025	3.7896	a	242.58
19	18	1	18	18	0	167 919.266	0.087	1.9474	a	265.73
19	3	17	18	3	16	167 928.560	0.052	18.5201	a	56.41
19	5	15	18	5	14	167 958.486	0.059	17.6845	a	67.07
19	5	14	18	5	13	167 966.243	0.046	17.6845	a	67.07
19	4	16	18	4	15	168 145.967	0.032	18.1573	a	61.09
19	4	15	18	4	14	168 323.612	0.070	18.1574	a	61.10
19	1	18	18	1	17	168 567.295	0.060	18.8695	a	51.91
20	0	20	19	0	19	169 576.957	0.018	19.9292	a	54.53
19	3	16	18	3	15	169 814.938	0.051	18.5260	a	56.60
19	2	17	18	2	16	171 704.487	0.012	18.7980	a	53.84
21	0	21	20	0	20	177 843.507	0.029	20.9283	a	60.18
11	3	9	10	2	8	194 144.997	0.022	3.8296	b	18.98
22	10	13	21	10	12	194205.395	0.020	17.4552	a	134.73
22	11	12	21	11	11	194 206.522	0.031	16.5007	a	148.72
23	1	23	22	1	22	194 209.226	–0.006	22.9252	a	72.35
23	0	23	22	0	22	194 390.209	0.038	22.9272	a	72.32
23	1	23	22	0	22	195 045.142	0.008	19.5185	b	72.32
20	2	19	19	1	18	195 507.658	0.010	9.4792	b	57.54
24	1	23	23	2	22	198 375.762	0.015	13.0370	b	83.20
27	2	25	26	3	24	198 645.870	0.012	8.5301	b	109.40
23	2	22	22	2	21	199 767.238	0.028	22.7827	a	76.54
23	1	22	22	1	21	201 840.134	0.026	22.8324	a	76.08
23	3	21	22	3	20	203 001.662	0.049	22.5939	a	80.58
23	11	12	22	11	11	203 036.102	0.053	17.7398	a	155.20
23	10	14	22	10	13	203 037.818	0.050	18.6529	a	141.21
23	12	11	22	12	10	203 045.656	0.040	16.7398	a	170.51
23	9	15	22	9	14	203 054.743	0.001	19.4790	a	128.55
23	13	10	22	13	9	203 064.000	0.011	15.6528	a	187.13
23	14	9	22	14	8	203 089.582	0.034	14.4788	a	205.08
23	8	16	22	8	15	203 093.710	0.049	20.2181	a	117.22
23	15	9	22	15	8	203 121.228	0.030	13.2179	a	224.33
23	16	7	22	16	6	203 158.166	–0.005	11.8700	a	244.89
23	7	17	22	7	16	203 166.635	0.042	20.8703	a	107.22
23	17	6	22	17	5	203 199.918	0.001	10.4352	a	266.75
23	18	6	22	18	5	203 245.984	–0.045	8.9134	a	289.90
23	19	5	22	19	4	203 296.106	–0.096	7.3046	a	314.35
23	6	18	22	6	17	203 296.757	0.066	21.4353	a	98.56
23	6	17	22	6	16	203 298.380	0.010	21.4353	a	98.56
23	20	3	22	20	2	203 350.082	–0.119	5.6089	a	340.09
23	21	2	22	21	1	203 407.712	–0.126	3.8262	a	367.11
23	22	2	22	22	1	203 468.787	–0.177	1.9566	a	395.41
23	5	19	22	5	18	203 519.398	0.020	21.9132	a	91.26
23	5	18	22	5	17	203 562.522	0.010	21.9132	a	91.26
23	4	20	22	4	19	203 734.137	0.019	22.3024	a	85.30
23	4	19	22	4	18	204 371.334	0.030	22.3031	a	85.35
23	3	20	22	3	19	206 899.456	0.020	22.6183	a	81.11
23	2	21	22	2	20	207 387.987	0.011	22.8143	a	78.54
26	2	25	25	2	24	225 056.930	0.004	25.7889	a	97.37
25	2	24	24	1	23	226 486.308	0.023	14.3041	b	89.82
27	1	27	26	1	26	227 451.904	–0.026	26.9254	a	99.93
27	0	27	26	0	26	227 521.640	–0.003	26.9260	a	99.92
26	3	24	25	3	23	229 074.738	–0.011	25.6288	a	101.76
26	5	21	25	5	20	230 375.077	0.000	25.0384	a	112.52
26	4	23	25	4	22	230 390.621	–0.006	25.3803	a	106.58
26	4	22	25	4	21	231 769.811	–0.011	25.3835	a	106.72
27	3	25	26	3	24	237 715.236	–0.009	26.6374	a	109.40
27	13	14	26	13	13	238 369.413	–0.010	20.7416	a	215.99
27	10	18	26	10	17	238 373.896	0.001	23.2972	a	170.07

Table 4. continued.

Transition						Obs. Freq.	obs.- calc.	S	Dipole	E_l
J'	K'_a	K'_c	J''	K''_a	K''_c	(MHz)	(MHz)			(cm^{-1})
27	14	14	26	14	13	238 392.400	–0.025	19.7415	a	233.94
27	9	19	26	9	18	238 414.308	0.018	24.0009	a	157.41
27	15	13	26	15	12	238 423.917	–0.012	18.6674	a	253.20
27	16	11	26	16	10	238 462.693	–0.010	17.5192	a	273.76
27	8	20	26	8	19	238 488.933	–0.015	24.6305	a	146.09
27	17	11	26	17	10	238 507.830	–0.036	16.2969	a	295.62
27	18	10	26	18	9	238 558.700	–0.069	15.0006	a	318.79
69	2	68	68	2	67	580 910.446	–0.040	68.7809	a	670.16
66	18	49	65	18	48	581 590.167	0.064	61.0945	a	846.84
66	17	50	65	17	49	581 601.544	0.080	61.6250	a	823.62
66	19	47	65	19	46	581612.441	0.049	60.5337	a	871.37
66	16	51	65	16	50	581 653.444	0.083	62.1252	a	801.73
66	20	46	65	20	45	581 663.189	0.001	59.9427	a	897.20
66	21	46	65	21	45	581 738.576	0.002	59.3213	a	924.34
66	15	52	65	15	51	581 755.324	0.090	62.5951	a	781.17
66	22	45	65	22	44	581 835.489	–0.029	58.6697	a	952.76
66	14	53	65	14	52	581 920.471	0.095	63.0347	a	761.95
66	23	43	65	23	42	581 951.567	–0.064	57.9877	a	982.47
66	24	43	65	24	42	582 085.039	0.029	57.2755	a	1013.46
66	13	54	65	13	53	582 168.249	0.097	63.4441	a	744.08
66	25	42	65	25	41	582 234.117	0.003	56.5329	a	1045.72
66	26	41	65	26	40	582 397.621	–0.060	55.7601	a	1079.24
66	12	55	65	12	54	582 528.138	0.179	63.8233	a	727.60
66	12	54	65	12	53	582 528.138	–0.032	63.8233	a	727.60
66	27	40	65	27	39	582 574.641	–0.026	54.9569	a	1114.02
66	28	38	65	28	37	582 764.214	0.017	54.1235	a	1150.05
66	29	37	65	29	36	582 965.647	0.117	53.2597	a	1187.32
66	11	56	65	11	55	583 046.157	0.076	64.1722	a	712.51
66	11	55	65	11	54	583 049.586	0.064	64.1722	a	712.51
66	10	57	65	10	56	583789.869	0.050	64.4909	a	698.87
66	10	56	65	10	55	583 834.239	0.052	64.4909	a	698.87
51	6	46	50	5	45	584 073.815	–0.027	11.7577	b	396.40
66	34	32	65	34	31	584129.722	0.017	48.4865	a	1392.05
67	4	63	66	4	62	584 286.076	0.000	66.4435	a	667.13
66	9	58	65	9	57	584 781.420	0.045	64.7788	a	686.71
66	7	60	65	7	59	584 876.867	0.007	65.2270	a	666.60
52	6	47	51	5	46	584 898.259	–0.129	12.1552	b	411.76
66	5	61	65	5	60	585 208.085	0.013	65.4062	a	656.63
66	9	57	65	9	56	585 212.206	0.065	64.7797	a	686.76
65	6	59	64	6	58	585 239.243	0.003	64.4771	a	643.49
68	4	65	67	4	64	585 447.928	–0.008	67.5358	a	675.77
68	3	65	67	3	64	585 488.461	–0.023	67.5360	a	675.77
53	6	48	52	5	47	585 590.283	0.007	12.6145	b	427.42
66	8	59	65	8	58	585 607.934	0.030	65.0310	a	676.05
68	4	65	67	3	64	585 648.728	–0.061	43.9222	b	675.77
54	6	49	53	5	48	586 212.150	0.079	13.1394	b	443.37
55	6	50	54	5	49	586 827.500	0.003	13.7327	b	459.61
67	5	63	66	4	62	586 869.571	0.021	34.9153	b	667.13
69	3	67	68	3	66	587 239.919	–0.069	68.6504	a	683.17
69	2	67	68	2	66	587 241.733	0.034	68.6504	a	683.17
69	3	67	68	2	66	587 247.796	0.000	52.1857	b	683.17
56	6	51	55	5	50	587 500.756	0.027	14.3964	b	476.14
57	6	52	56	5	51	588 295.528	0.001	15.1314	b	492.96
66	8	58	65	8	57	588 408.553	0.014	65.0432	a	676.47
70	1	69	69	1	68	589 128.465	–0.035	69.7809	a	689.54
58	6	53	57	5	52	589 274.098	–0.010	15.9372	b	510.06
38	7	32	37	6	31	590 245.915	–0.041	11.1457	b	231.48
59	6	54	58	5	53	590 495.691	–0.074	16.8118	b	527.43
42	6	36	41	5	37	590 793.431	–0.028	9.5155	b	271.07
71	0	71	70	0	70	591 053.717	–0.053	70.9244	a	694.96
69	5	64	68	6	63	591 221.099	0.125	27.7557	b	716.57
38	7	31	37	6	32	591 382.017	–0.044	11.1348	b	231.45
68	5	64	67	5	63	591 943.537	–0.014	67.4378	a	686.70
60	6	55	59	5	54	592 015.086	–0.150	17.7513	b	545.08
68	4	64	67	4	63	592 409.523	0.006	67.4410	a	686.62

Table 4. continued.

Transition						Obs. Freq.	obs.- calc.	S	Dipole	E_l
J'	K'_a	K'_c	J''	K''_a	K''_c	(MHz)	(MHz)			(cm^{-1})
69	3	66	68	4	65	593 526.217	–0.034	44.9453	b	695.30
69	4	66	68	4	65	593 654.043	–0.010	68.5348	a	695.30
42	5	37	41	4	38	593 661.871	–0.044	5.3642	b	264.67
66	6	60	65	6	59	593 732.907	0.000	65.4689	a	663.02
69	4	66	68	3	65	593 814.241	–0.117	44.9464	b	695.30
66	7	59	65	7	58	593 850.986	0.006	65.3278	a	668.70
61	6	56	60	5	55	593 880.970	0.009	18.7503	b	563.00
70	2	68	69	3	67	595 447.285	–0.015	53.1906	b	702.76
70	3	68	69	3	67	595 452.017	–0.042	69.6501	a	702.76
70	2	68	69	2	67	595 453.457	0.060	69.6501	a	702.76
70	3	68	69	2	67	595 458.219	0.063	53.1906	b	702.76
71	1	70	70	1	69	597 343.930	–0.006	70.7808	a	709.19
39	7	33	38	6	32	598 252.929	–0.042	11.2494	b	242.74
69	4	65	68	5	64	598 423.836	0.228	37.0595	b	706.45
63	6	58	62	5	57	598 803.592	0.107	20.8977	b	599.65
39	7	32	38	6	33	599 792.633	–0.123	11.2341	b	242.69
68	5	63	67	5	62	601 035.254	0.012	67.3869	a	695.93
43	6	37	42	5	38	601 215.210	–0.063	9.3866	b	283.49
70	3	67	69	4	66	601 755.785	0.046	45.9678	b	715.10
70	5	65	69	6	64	601 828.584	0.016	28.9717	b	736.79
70	4	67	69	4	66	601 857.553	0.030	69.5339	a	715.10
70	3	67	69	3	66	601 883.555	0.014	69.5340	a	715.10
64	6	59	63	5	58	601 911.925	0.051	22.0290	b	618.38
70	4	67	69	3	66	601 985.414	0.089	45.9687	b	715.10
71	2	69	70	3	68	603 657.935	–0.008	54.1948	b	722.62
71	3	69	70	3	68	603 661.656	0.001	70.6497	a	722.62
71	2	69	70	2	68	603 662.751	0.050	70.6497	a	722.62
71	3	69	70	2	68	603 666.473	0.059	54.1948	b	722.62
70	9	62	69	9	61	620 433.510	–0.042	68.8496	a	766.52
70	9	61	69	9	60	621 434.243	0.074	68.8524	a	766.65
23	11	13	22	10	12	622 356.554	–0.065	11.9564	b	141.21
71	6	66	70	6	65	622 852.683	–0.044	70.3468	a	757.29
45	6	39	44	5	40	623 459.775	0.033	9.0142	b	309.21
69	6	64	68	5	63	624 029.166	0.010	27.9286	b	715.98
37	8	29	36	7	30	624 272.377	–0.087	12.0107	b	229.03
71	5	66	70	5	65	624 852.289	–0.016	70.3661	a	756.87
42	7	35	41	6	36	625 048.068	–0.035	11.4760	b	278.20
71	18	54	70	18	53	625 329.473	–0.017	66.4409	a	946.75
71	19	52	70	19	51	625 331.305	0.008	65.9196	a	971.29
71	20	51	70	20	50	625 366.960	–0.103	65.3701	a	997.13
71	17	55	70	17	54	625 368.104	0.030	66.9341	a	923.54
71	21	50	70	21	49	625 431.838	–0.073	64.7924	a	1024.28
71	16	56	70	16	55	625 455.718	0.008	67.3992	a	901.66
71	22	49	70	22	48	625 522.002	–0.073	64.1866	a	1052.72
71	15	57	70	15	56	625 604.365	0.016	67.8361	a	881.12
71	23	48	70	23	47	625 634.526	–0.075	63.5526	a	1082.45
71	24	48	70	24	47	625 767.015	–0.119	62.8905	a	1113.46
71	14	58	70	14	57	625 830.991	0.011	68.2449	a	861.93
71	25	46	70	25	45	625 917.915	0.136	62.2002	a	1145.74
71	26	46	70	26	45	626 084.975	–0.011	61.4818	a	1179.29
71	13	59	70	13	58	626 160.719	0.038	68.6256	a	844.12
71	27	45	70	27	44	626 267.465	–0.008	60.7351	a	1214.10
71	28	44	70	28	43	626 464.214	0.043	59.9603	a	1250.16
71	12	60	70	12	59	626 631.955	–0.085	68.9782	a	827.70
19	12	7	18	11	8	626 633.366	–0.061	12.1192	b	131.05
28	10	19	27	9	18	626 647.471	–0.080	12.0899	b	165.36
71	11	61	70	11	60	627 304.657	–0.009	69.3029	a	812.71
71	11	60	70	11	59	627 318.951	–0.004	69.3029	a	812.71
71	7	65	70	7	64	627 682.434	–0.014	70.2488	a	767.01
71	10	62	70	10	61	628 244.441	–0.018	69.5994	a	799.20
71	10	61	70	10	60	628 398.854	–0.040	69.5997	a	799.22
44	5	39	43	4	40	628 804.286	–0.033	4.6167	b	289.62
71	9	63	70	9	62	629 334.548	–0.091	69.8660	a	787.22
70	6	65	69	5	64	629 649.968	0.036	29.1123	b	736.29
71	8	64	70	8	63	629 689.722	–0.060	70.0910	a	776.67
33	9	25	32	8	24	630 376.058	0.053	12.2129	b	198.25

Table 4. continued.

Transition						Obs. Freq.	obs.- calc.	S	Dipole	E_l
J'	K_a'	K_c'	J''	K_a''	K_c''	(MHz)	(MHz)			(cm^{-1})
71	9	62	70	9	61	630 551.511	–0.072	69.8696	a	787.38
24	11	14	23	10	13	631 184.572	–0.134	12.1283	b	147.98
38	8	31	37	7	30	632 719.694	–0.025	12.1516	b	239.95
43	7	36	42	6	37	633 515.496	0.101	11.5345	b	290.63
71	6	65	70	6	64	634 830.982	–0.083	70.3972	a	764.81
29	10	20	28	9	19	635 436.249	–0.110	12.2695	b	173.61
71	8	63	70	8	62	635 441.009	–0.144	70.1353	a	777.74
20	12	8	19	11	9	635 476.076	0.012	12.2624	b	136.65
71	6	66	70	5	65	635 604.795	0.065	30.2881	b	756.87
44	7	38	43	6	37	635 916.160	0.123	11.6547	b	303.54
71	7	64	70	7	63	639 565.168	–0.109	70.3990	a	770.82
16	13	4	15	12	3	639 601.580	0.158	12.6393	b	131.34
25	11	15	24	10	14	640 009.763	–0.068	12.3026	b	155.05
39	8	32	38	7	31	641 178.007	–0.083	12.2879	b	251.18
44	7	37	43	6	38	642 034.932	–0.047	11.5799	b	303.36
45	7	39	44	6	38	642 777.162	0.135	11.7116	b	316.62
21	12	9	20	11	10	644 317.823	0.032	12.4127	b	142.54

Table 5. Measured transitions of the ground vibrational state of CH_2DCH_2CN in-plane.

Transition						Obs. Freq.	obs.- calc.	S	Dipole	E_l
J'	K'_a	K'_c	J''	K''_a	K''_c	(MHz)	(MHz)			(cm^{-1})
1	0	1	0	0	0	8425.939	0.007	1.0000	a	0.00
32	4	28	32	4	29	8545.382	0.014	0.8744	a	161.32
6	1	5	6	1	6	8904.345	0.033	0.3101	a	6.53
17	4	14	18	3	15	9080.706	0.031	2.8265	b	55.26
14	2	12	14	2	13	9580.530	0.060	0.5108	a	32.58
12	1	12	11	2	9	9611.583	–0.026	1.2987	b	21.79
23	3	20	23	3	21	9736.492	–0.005	0.6882	a	84.74
12	3	9	13	2	12	9782.272	0.007	1.9814	b	28.66
20	3	17	19	4	16	9797.651	0.072	3.2576	b	65.98
28	6	23	29	5	24	10 435.821	–0.013	4.5950	b	142.03
33	4	29	33	4	30	10 622.685	0.009	0.8338	a	170.63
28	6	22	29	5	25	10 708.261	–0.015	4.5938	b	142.02
26	4	23	25	5	20	10 770.702	0.000	4.2252	b	111.02
7	2	5	8	1	8	11 443.994	0.038	1.0495	b	10.64
4	0	4	3	1	3	11 454.930	0.027	1.6021	b	2.43
25	1	25	24	2	22	11 654.174	0.062	0.4494	b	88.83
17	4	13	18	3	16	11 657.283	–0.019	2.8064	b	55.17
7	1	6	7	1	7	11 866.812	0.033	0.2688	a	8.45
11	3	9	12	2	10	11 986.814	0.025	1.8506	b	25.20
24	3	21	24	3	22	12 193.569	0.020	0.6475	a	91.50
15	2	13	15	2	14	12 241.041	0.000	0.4694	a	36.78
16	2	15	15	3	12	12 542.290	0.014	2.4780	b	40.84
26	4	22	25	5	21	12 675.233	0.025	4.2381	b	111.02
21	3	19	20	4	16	13 372.339	–0.008	3.4040	b	71.63
13	1	13	12	2	10	13 582.502	–0.037	1.2830	b	25.20
22	5	18	23	4	19	14 491.445	0.026	3.6010	b	90.25
9	1	8	8	2	7	14 745.126	0.041	1.8066	b	13.24
33	7	27	34	6	28	15 053.256	0.072	5.3741	b	195.64
25	3	22	25	3	23	15 067.335	0.051	0.6093	a	98.54
24	1	24	23	2	21	15 191.807	0.022	0.4994	b	81.94
22	5	17	23	4	20	15 230.412	–0.010	3.5970	b	90.22
8	1	7	8	1	8	15 246.729	0.046	0.2375	a	10.64
16	2	14	16	2	15	15 330.827	0.016	0.4328	a	41.26
5	2	4	6	1	5	15 373.653	0.029	0.9039	b	6.83
2	1	2	1	1	1	16 427.722	0.024	1.5000	a	1.06
2	0	2	1	0	1	16 846.054	0.011	1.9999	a	0.28
14	1	14	13	2	11	16 958.901	–0.021	1.2422	b	28.91
2	1	1	1	1	0	17 276.280	0.012	1.5000	a	1.07
1	1	0	1	0	1	23 650.020	0.017	1.5000	b	0.28
2	1	1	2	0	2	24 080.240	0.012	2.4773	b	0.84
3	0	3	2	0	2	25 254.560	0.039	2.9995	a	0.84
3	2	2	2	2	1	25 278.710	0.078	1.6667	a	3.97
3	2	1	2	2	0	25 301.600	–0.061	1.6667	a	3.97
1	1	1	0	0	0	31 651.640	0.003	1.0000	b	0.00
2	1	2	1	0	1	39 653.410	0.007	1.5000	b	0.28
18	8	10	17	8	9	151 816.716	0.004	14.4447	a	93.00
18	7	11	17	7	10	151 820.214	–0.005	15.2781	a	81.30
18	9	9	17	9	8	151 825.243	–0.018	13.5003	a	106.25
18	6	12	17	6	11	151 842.455	–0.022	16.0003	a	71.16
18	6	13	17	6	12	151 842.455	–0.005	16.0003	a	71.16
18	10	8	17	10	7	151 842.455	0.026	12.4447	a	121.05
18	11	7	17	11	6	151 866.350	0.055	11.2780	a	137.39
18	12	6	17	12	5	151 895.744	0.031	10.0002	a	155.27
18	5	14	17	5	13	151 897.570	0.028	16.6113	a	62.57
18	5	13	17	5	12	151 898.638	0.032	16.6113	a	62.58
18	13	5	17	13	4	151 929.957	–0.004	8.6113	a	174.68
18	14	4	17	14	3	151 968.645	0.081	7.1113	a	195.62
18	3	15	17	3	14	152 702.039	0.048	17.4987	a	50.16
18	1	17	17	1	16	153 673.504	0.049	17.9123	a	44.64
18	2	16	17	2	15	154 704.840	0.027	17.7843	a	46.64
19	1	19	18	1	18	154 817.517	0.020	18.9325	a	47.44
19	0	19	18	0	18	155 545.395	0.016	18.9457	a	47.29
19	8	11	18	8	10	160 254.462	0.025	15.6319	a	98.06
19	9	10	18	9	9	160 261.323	0.123	14.7371	a	111.31
19	10	9	18	10	8	160 277.669	–0.045	13.7371	a	126.11

Table 5. continued.

Transition						Obs. Freq.	obs.- calc.	S	Dipole	E_l
J'	K'_a	K'_c	J''	K''_a	K''_c	(MHz)	(MHz)			(cm^{-1})
19	6	13	18	6	12	160 290.086	–0.091	17.1055	a	76.22
19	6	14	18	6	13	160 290.086	–0.059	17.1055	a	76.22
19	11	8	18	11	7	160 301.741	0.021	12.6318	a	142.46
19	5	15	18	5	14	160 356.951	0.051	17.6844	a	67.64
19	5	14	18	5	13	160 358.615	–0.027	17.6844	a	67.64
19	13	6	18	13	5	160 367.315	–0.003	10.1055	a	179.75
19	3	17	18	3	16	160 449.332	0.060	18.5237	a	55.17
19	15	4	18	15	3	160 452.111	0.057	7.1580	a	223.16
19	4	15	18	4	14	160 537.921	0.058	18.1577	a	60.63
19	3	16	18	3	15	161 345.884	0.054	18.5249	a	55.26
19	1	18	18	1	17	161 950.886	0.080	18.9087	a	49.77
20	1	20	19	1	19	162 866.536	0.064	19.9336	a	52.60
19	2	17	18	2	16	163 411.936	0.025	18.7971	a	51.80
20	0	20	19	0	19	163 495.889	–0.003	19.9439	a	52.47
20	1	20	19	0	19	166 695.718	0.052	15.7189	b	52.47
20	2	19	19	2	18	167 236.798	0.009	19.7835	a	56.34
20	3	18	19	3	17	168 887.115	0.127	19.5468	a	60.52
20	15	5	19	15	4	168 892.325	0.098	8.7502	a	228.51
20	3	17	19	3	16	170 019.778	–0.002	19.5486	a	60.64
20	1	19	19	1	18	170 181.782	–0.031	19.9040	a	55.17
21	1	21	20	1	20	170 907.425	0.067	20.9345	a	58.03
21	0	21	20	0	20	171 446.582	–0.018	20.9424	a	57.93
20	2	18	19	2	17	172 097.307	0.044	19.8083	a	57.25
21	2	20	20	2	19	175 465.883	0.074	20.7906	a	61.92
22	0	22	21	1	21	176 738.576	0.041	17.7252	b	63.74
21	8	14	20	8	13	177 131.593	0.028	17.9527	a	109.04
21	9	13	20	9	12	177 133.673	0.027	17.1432	a	122.29
21	7	15	20	7	14	177 147.302	0.021	18.6670	a	97.34
21	7	14	20	7	13	177 147.302	0.020	18.6670	a	97.34
21	10	12	20	10	11	177 148.099	0.038	16.2384	a	137.09
21	11	11	20	11	10	177 171.763	0.001	15.2384	a	153.43
21	6	15	20	6	14	177 191.500	–0.014	19.2860	a	87.20
21	6	16	20	6	15	177 191.500	0.084	19.2860	a	87.20
21	12	10	20	12	9	177 202.931	–0.003	14.1431	a	171.31
21	13	9	20	13	8	177 240.454	0.017	12.9526	a	190.73
21	14	8	20	14	7	177 283.518	–0.004	11.6669	a	211.68
21	5	17	20	5	16	177 285.473	0.003	19.8097	a	78.62
21	5	16	20	5	15	177 289.764	–0.022	19.8097	a	78.62
21	3	19	20	3	18	177 316.693	0.021	20.5674	a	66.16
21	15	7	20	15	6	177 331.714	0.035	10.2859	a	234.14
21	16	6	20	16	5	177 384.553	0.005	8.8097	a	258.13
21	1	20	20	1	19	178 365.373	–0.023	20.8985	a	60.85
21	3	18	20	3	17	178 723.953	–0.049	20.5702	a	66.31
22	1	22	21	1	21	178 940.860	0.017	21.9351	a	63.74
24	1	23	23	2	22	179 076.241	0.050	10.9652	b	80.30
22	0	22	21	0	21	179 399.072	0.005	21.9413	a	63.65
21	2	19	20	2	18	180 756.379	–0.052	20.8178	a	62.99
23	0	23	22	1	22	185 151.896	0.009	18.7616	b	69.70
22	8	15	21	8	14	185 571.039	0.017	19.0913	a	114.94
22	10	13	21	10	12	185 583.103	–0.007	17.4549	a	143.00
22	7	16	21	7	15	185 591.954	–0.006	19.7731	a	103.25
22	7	15	21	7	14	185 591.954	–0.009	19.7731	a	103.25
22	11	12	21	11	11	185 606.338	–0.011	16.5003	a	159.34
22	12	11	21	12	10	185 637.799	0.003	15.4549	a	177.22
22	6	16	21	6	15	185 645.289	–0.078	20.3639	a	93.11
22	6	17	21	6	16	185 645.289	0.087	20.3639	a	93.11
22	13	10	21	13	9	185 676.153	0.011	14.3185	a	196.64
22	14	9	21	14	8	185 720.533	0.003	13.0912	a	217.59
22	3	20	21	3	19	185 736.901	–0.018	21.5859	a	72.07
22	5	18	21	5	17	185 754.911	0.006	20.8637	a	84.54
22	5	17	21	5	16	185 761.477	0.004	20.8637	a	84.54
22	16	7	21	16	6	185 825.261	0.001	10.3638	a	264.05
22	4	19	21	4	18	185 926.787	–0.011	21.2722	a	77.54
22	4	18	21	4	17	186 081.659	0.011	21.2722	a	77.55
22	1	21	21	1	20	186 501.648	–0.012	21.8923	a	66.80
22	3	19	21	3	18	187 457.424	–0.021	21.5902	a	72.27

Table 5. continued.

Transition						Obs. Freq.	obs.- calc.	S	Dipole	E_l
J'	K'_a	K'_c	J''	K''_a	K''_c	(MHz)	(MHz)			(cm^{-1})
22	2	20	21	2	19	189 385.671	0.047	21.8258	a	69.02
24	1	24	23	1	23	194 988.303	0.023	23.9360	a	75.94
24	0	24	23	0	23	195 312.455	0.063	23.9397	a	75.88
24	2	23	23	2	22	200 052.012	0.039	23.8063	a	80.30
26	1	25	25	2	24	200 081.553	–0.025	12.9565	b	93.91
31	5	26	31	4	27	201 686.898	0.019	17.2825	b	152.52
20	2	19	19	1	18	202 187.049	–0.009	8.3245	b	55.17
24	9	16	23	9	15	202 443.823	–0.017	20.6254	a	140.86
24	8	17	23	8	16	202 451.840	–0.010	21.3337	a	127.61
24	10	15	23	10	14	202 452.935	0.004	19.8337	a	155.66
24	11	14	23	11	13	202 474.550	–0.025	18.9587	a	172.00
24	7	18	23	7	17	202 485.124	–0.015	21.9587	a	115.91
24	7	17	23	7	16	202 485.124	–0.023	21.9587	a	115.91
24	12	13	23	12	12	202 506.079	0.015	18.0004	a	189.89
24	3	22	23	3	21	202 543.673	–0.023	23.6176	a	84.74
24	13	12	23	13	11	202 545.683	–0.020	16.9587	a	209.31
24	14	11	23	14	10	202 592.374	–0.006	15.8337	a	230.26
24	1	23	23	1	22	202 639.497	–0.001	23.8787	a	79.51
24	15	10	23	15	9	202 645.341	0.000	14.6253	a	252.73
24	5	19	23	5	18	202 718.796	–0.011	22.9584	a	97.21
24	17	8	23	17	7	202 768.148	0.013	11.9586	a	302.23
24	18	7	23	18	6	202 837.343	0.045	10.5002	a	329.23
24	4	21	23	4	20	202 900.357	–0.010	23.3324	a	90.22
25	1	25	24	1	24	203 003.517	0.027	24.9363	a	82.44
30	5	25	30	4	26	203 112.867	0.026	16.5933	b	143.72
24	4	20	23	4	19	203 179.468	–0.001	23.3326	a	90.25
25	0	25	24	0	24	203 273.733	0.019	24.9392	a	82.40
24	3	21	23	3	20	205 000.790	0.042	23.6264	a	85.07
24	2	22	23	2	21	206 541.142	–0.020	23.8372	a	81.94
21	2	20	20	1	19	207 471.062	0.008	9.0389	b	60.85
25	5	20	25	4	21	207 737.141	–0.012	13.3359	b	104.09
33	5	29	33	4	30	207 894.128	0.048	18.3967	b	170.63
32	5	28	32	4	29	207 911.479	0.039	17.7510	b	161.32
34	5	30	34	4	31	207 945.427	0.035	19.0420	b	180.23
31	5	27	31	4	28	207 985.320	–0.001	17.1064	b	152.29
35	5	31	35	4	32	208 078.135	0.013	19.6854	b	190.10
25	2	24	24	2	23	208 214.052	–0.009	24.8099	a	86.97
29	5	25	29	4	26	208 257.868	–0.005	15.8248	b	135.08
24	5	19	24	4	20	208 286.349	–0.001	12.7126	b	97.03
36	5	32	36	4	33	208 305.463	0.007	20.3251	b	200.25
26	5	22	26	4	23	208 835.101	0.013	13.9326	b	111.38
25	5	21	25	4	22	209 041.286	–0.007	13.3116	b	104.04
22	5	17	22	4	18	209 131.839	–0.010	11.4872	b	83.76
23	5	19	23	4	20	209 440.416	–0.014	12.0853	b	90.22
22	5	18	22	4	19	209 625.542	–0.044	11.4796	b	83.74
20	5	15	20	4	16	209 717.249	0.009	10.2853	b	71.63
21	5	17	21	4	18	209 797.456	–0.023	10.8786	b	77.54
19	5	14	19	4	15	209 935.869	0.001	9.6913	b	65.99
26	0	26	25	1	25	210 016.606	–0.005	21.8503	b	89.22
19	5	15	19	4	16	210 095.346	0.020	9.6893	b	65.98
18	5	13	18	4	14	210 115.114	0.026	9.1011	b	60.63
18	5	14	18	4	15	210 219.904	0.024	9.0998	b	60.63
27	1	26	26	2	25	210 292.455	–0.022	13.9945	b	101.13
16	5	11	16	4	12	210 378.953	0.019	7.9283	b	50.77
16	5	12	16	4	13	210 420.751	–0.002	7.9279	b	50.77
40	5	36	40	4	37	210 429.828	–0.009	22.8052	b	243.67
15	5	10	15	4	11	210 473.249	0.004	7.3438	b	46.27
15	5	11	15	4	12	210 498.484	0.011	7.3436	b	46.27
25	1	24	24	1	23	210 648.123	–0.020	24.8718	a	86.27
25	9	17	24	9	16	210 880.985	–0.020	21.7604	a	147.61
25	10	16	24	10	15	210 887.671	–0.019	21.0004	a	162.41
25	8	18	24	8	17	210 893.254	–0.019	22.4404	a	134.36
25	11	15	24	11	14	210 908.154	–0.028	20.1604	a	178.76
25	3	23	24	3	22	210 927.693	0.006	24.6312	a	91.50
25	12	14	24	12	13	210 939.426	0.002	19.2404	a	196.65

Table 5. continued.

Transition						Obs. Freq.	obs.- calc.	S	Dipole	E_l
J'	K'_a	K'_c	J''	K''_a	K''_c	(MHz)	(MHz)			(cm^{-1})
25	13	13	24	13	12	210 979.468	–0.032	18.2404	a	216.07
26	1	26	25	1	25	211 013.830	0.034	25.9365	a	89.22
25	6	20	24	6	19	211 020.394	0.052	23.5603	a	112.53
25	6	19	24	6	18	211 020.971	–0.052	23.5603	a	112.53
25	14	12	24	14	11	211 027.168	0.012	17.1604	a	237.02
25	15	11	24	15	10	211 081.509	–0.032	16.0003	a	259.49
25	16	10	24	16	9	211 142.064	0.008	14.7603	a	283.49
25	5	21	24	5	20	211 184.622	–0.035	24.0000	a	103.97
25	5	20	24	5	19	211 205.283	–0.018	24.0000	a	103.97
25	17	9	24	17	8	211 208.264	–0.005	13.4403	a	308.99
26	0	26	25	0	25	211 238.030	0.041	25.9387	a	89.18
25	18	8	24	18	7	211 279.860	0.001	12.0402	a	336.00
25	19	7	24	19	6	211 356.596	0.014	10.5602	a	364.50
25	4	22	24	4	21	211 387.864	–0.030	24.3588	a	96.99
25	4	21	24	4	20	211 754.476	–0.023	24.3591	a	97.03
27	0	27	26	0	26	219 204.852	–0.057	26.9384	a	96.22
26	3	23	25	3	22	222 613.281	0.024	25.6590	a	99.04
48	5	44	48	4	45	223 018.116	–0.020	26.9241	b	343.77
24	2	23	23	1	22	223 615.262	–0.017	11.4810	b	79.51
27	2	26	26	2	25	224 490.154	–0.026	26.8155	a	101.13
49	5	45	49	4	46	225 548.261	–0.037	27.3242	b	357.52
27	1	26	26	1	25	226 570.969	0.095	26.8590	a	100.59
27	3	25	26	3	24	227 651.138	–0.050	26.6543	a	105.85
27	11	16	26	11	15	227 774.221	–0.083	22.5190	a	193.11
27	8	19	26	8	18	227 778.208	–0.060	24.6301	a	148.71
27	7	20	26	7	19	227 835.241	–0.087	25.1856	a	137.02
27	7	21	26	7	20	227 835.241	–0.046	25.1856	a	137.02
27	13	14	26	13	13	227 845.024	0.042	20.7412	a	230.42
27	15	12	26	15	11	227 951.108	–0.081	18.6670	a	273.86
27	6	21	26	6	20	227 951.108	–0.023	25.6670	a	126.89
27	5	23	26	5	22	228 155.714	0.011	26.0740	a	118.34
27	5	22	26	5	21	228 196.540	–0.028	26.0740	a	118.35
27	4	23	26	4	22	228 967.170	–0.119	26.4062	a	111.44
27	3	24	26	3	23	231 429.068	0.022	26.6743	a	106.46
27	2	25	26	2	24	231 974.973	–0.012	26.8428	a	103.46
28	1	27	27	1	26	234 497.116	–0.059	27.8534	a	108.15
26	2	25	25	1	24	234 901.664	–0.011	13.3303	b	93.30
29	1	29	28	1	28	235 020.178	0.017	28.9368	a	111.13
29	0	29	28	0	28	235 145.122	–0.006	28.9378	a	111.11
28	9	19	27	9	18	236 193.848	–0.048	25.1076	a	169.56
28	11	17	27	11	16	236 206.674	–0.110	23.6791	a	200.71
28	12	16	27	12	15	236 236.176	0.052	22.8576	a	218.60
28	13	15	27	13	14	236 276.598	–0.011	21.9647	a	238.02
28	7	21	27	7	20	236 288.325	–0.070	26.2504	a	144.62
28	7	22	27	7	21	236 288.325	–0.004	26.2504	a	144.62
28	14	14	27	14	13	236 326.451	–0.035	21.0004	a	258.98
28	2	26	27	2	25	240 362.646	0.007	27.8417	a	111.20
29	9	20	28	9	19	244 631.909	–0.103	26.2074	a	177.44
29	11	18	28	11	17	244 638.822	–0.034	24.8281	a	208.59
29	13	16	28	13	15	244 707.482	0.027	23.1729	a	245.91
29	5	24	28	5	23	245 216.694	–0.042	28.1378	a	133.85
29	2	27	28	2	26	248 701.154	–0.076	28.8392	a	119.21
29	3	26	28	3	25	249 042.252	–0.028	28.7027	a	122.20
71	3	69	70	2	68	581 731.107	0.002	50.9583	b	696.18
69	10	60	68	10	59	581 801.782	0.012	67.5542	a	738.00
69	10	59	68	10	58	581 806.439	–0.045	67.5542	a	738.00
18	13	6	18	12	7	582 029.164	–0.023	5.0897	b	160.34
19	13	7	19	12	8	582 064.607	–0.027	5.8179	b	165.68
22	13	10	22	12	11	582 177.124	0.106	7.8913	b	183.42
69	9	60	68	9	59	582 505.572	0.021	67.8299	a	723.50
59	13	46	59	12	47	582 556.178	–0.016	30.0532	b	610.11
57	13	44	57	12	45	582 683.177	0.033	28.8600	b	577.22
35	13	22	35	12	23	582 685.666	0.032	15.9398	b	289.51
56	13	44	56	12	45	582 735.651	0.019	28.2657	b	561.20
37	13	25	37	12	26	582 751.975	0.000	17.1194	b	310.05

Table 5. continued.

		Transition				Obs. Freq.	obs.- calc.	S	Dipole	E_l
J'	K'_a	K'_c	J''	K''_a	K''_c	(MHz)	(MHz)			(cm^{-1})
51	13	39	51	12	40	582 900.732	–0.045	25.3134	b	485.28
44	13	32	44	12	33	582 912.908	–0.005	21.2162	b	390.79
50	13	38	50	12	39	582 916.474	0.016	24.7262	b	470.94
45	13	33	45	12	34	582923.809	0.024	21.8003	b	403.45
49	13	36	49	12	37	582 926.975	–0.059	24.1398	b	456.88
68	6	62	67	6	61	583 163.419	0.014	67.5275	a	673.26
69	8	61	68	8	60	583 883.560	0.048	68.0770	a	710.80
73	1	73	72	1	72	584 970.291	–0.010	72.9362	a	707.49
73	0	73	72	0	72	584 970.291	–0.016	72.9362	a	707.49
70	5	66	69	5	65	586 112.852	0.002	69.5382	a	699.36
17	10	8	16	9	7	587 026.949	–0.003	10.2347	b	101.47
17	10	7	16	9	8	587 026.949	–0.003	10.2347	b	101.47
69	7	62	68	7	61	587 335.352	0.017	68.3032	a	700.29
71	4	68	70	4	67	587 989.515	–0.005	70.6170	a	708.11
71	3	68	70	3	67	588 216.282	–0.009	70.6183	a	708.06
70	4	66	69	4	65	588 230.948	–0.028	69.5588	a	698.83
70	15	56	69	15	55	589 198.839	0.026	66.7881	a	854.26
70	16	55	69	16	54	589 220.285	–0.011	66.3451	a	878.35
70	14	57	69	14	56	589 227.181	–0.010	67.2026	a	831.72
70	17	54	69	17	53	589 282.589	0.029	65.8735	a	903.98
70	13	58	69	13	57	589 318.443	–0.020	67.5885	a	810.75
70	18	53	69	18	52	589 379.100	0.016	65.3734	a	931.13
69	5	64	68	5	63	589 476.394	0.012	68.5973	a	686.84
70	12	59	69	12	58	589 492.053	0.018	67.9459	a	791.35
70	12	58	69	12	57	589 492.053	0.000	67.9459	a	791.35
70	19	52	69	19	51	589 505.077	0.009	64.8447	a	959.81
72	3	70	71	3	69	589 547.823	–0.018	71.7088	a	715.58
72	2	70	71	2	69	589 560.420	–0.008	71.7088	a	715.58
70	20	51	69	20	50	589 656.905	0.003	64.2875	a	990.00
70	21	50	69	21	49	589 831.784	–0.033	63.7017	a	1021.68
70	22	49	69	22	48	590 027.647	–0.007	63.0873	a	1054.86
70	10	61	69	10	60	590 225.004	0.031	68.5750	a	757.40
70	10	60	69	10	59	590 231.067	0.011	68.5751	a	757.40
70	23	48	69	23	47	590 242.680	–0.023	62.4443	a	1089.51
70	24	47	69	24	46	590 475.568	–0.020	61.7728	a	1125.64
70	6	65	69	6	64	590 514.222	0.008	69.4441	a	709.16
70	25	46	69	25	45	590 725.141	–0.046	61.0727	a	1163.23
70	9	62	69	9	61	590 897.085	–0.040	68.8468	a	742.92
70	9	61	69	9	60	590 974.749	0.002	68.8469	a	742.93
12	11	2	11	10	1	591 017.927	0.015	10.5274	b	96.57
12	11	1	11	10	2	591 017.927	0.015	10.5274	b	96.57
23	9	14	22	8	15	591 272.704	–0.030	10.5432	b	121.13
70	7	64	69	7	63	592 141.887	0.021	69.2948	a	719.08
70	8	62	69	8	61	592 473.051	0.026	69.0907	a	730.28
74	1	74	73	1	73	592 876.923	–0.008	73.9362	a	727.00
74	0	74	73	0	73	592 876.923	–0.013	73.9362	a	727.00
71	5	67	70	5	66	594 080.307	–0.004	70.5376	a	718.91
29	8	22	28	7	21	595 063.200	0.006	10.9636	b	152.50
18	10	8	17	9	9	595 479.907	0.025	10.3954	b	106.25
18	10	9	17	9	8	595 479.907	0.025	10.3954	b	106.25
72	4	69	71	4	68	595 890.098	0.003	71.6161	a	727.72
71	4	67	70	4	66	595 949.234	0.015	70.5547	a	718.45
70	7	63	69	7	62	596 200.522	0.040	69.3164	a	719.88
70	5	65	69	5	64	597 381.982	0.007	69.5871	a	706.50
73	2	71	72	3	70	597 400.251	–0.031	52.9773	b	735.25
73	3	71	72	3	70	597 446.669	0.010	72.7084	a	735.25
73	2	71	72	2	70	597 456.985	0.000	72.7085	a	735.25
71	15	57	70	15	56	597 553.967	0.015	67.8335	a	873.91
71	16	56	70	16	55	597 571.045	0.005	67.3967	a	898.00
71	14	58	70	14	57	597 588.549	0.016	68.2421	a	851.38
71	17	55	70	17	54	597 630.313	0.008	66.9318	a	923.63
71	13	59	70	13	58	597 688.446	0.022	68.6226	a	830.41
71	18	54	70	18	53	597 724.959	0.018	66.4387	a	950.79
71	19	53	70	19	52	597 849.948	0.007	65.9174	a	979.47
71	12	60	70	12	59	597 873.990	0.013	68.9750	a	811.02
71	12	59	70	12	58	597 873.990	–0.011	68.9750	a	811.02

Table 5. continued.

Transition						Obs. Freq.	obs.- calc.	S	Dipole	E_l
J'	K'_a	K'_c	J''	K''_a	K''_c	(MHz)	(MHz)			(cm^{-1})
71	20	52	70	20	51	598 001.604	0.063	65.3680	a	1009.66
71	22	50	70	22	49	598 373.637	–0.006	64.1847	a	1074.54
71	23	49	70	23	48	598 590.108	–0.007	63.5508	a	1109.20
71	10	62	70	10	61	598 647.897	0.034	69.5954	a	777.09
71	10	61	70	10	60	598 655.695	0.018	69.5954	a	777.09
71	6	66	70	6	65	598 671.285	0.026	70.4468	a	728.85
71	24	48	70	24	47	598 824.816	–0.027	62.8887	a	1145.34
71	9	63	70	9	62	599 350.867	0.009	69.8633	a	762.63
71	9	62	70	9	61	599 447.258	–0.054	69.8635	a	762.65
13	11	2	12	10	3	599 474.189	0.011	10.5910	b	99.94
13	11	3	12	10	2	599 474.189	0.011	10.5910	b	99.94
24	9	16	23	8	15	599 705.411	–0.055	10.7335	b	127.61
16	14	3	16	13	4	627 769.897	–0.056	2.7574	b	169.90
17	14	4	17	13	5	627 806.870	–0.015	3.5832	b	174.68
19	14	6	19	13	7	627 885.681	0.005	5.1385	b	185.10
21	14	8	21	13	9	627 970.385	–0.060	6.5965	b	196.64
23	14	10	23	13	11	628 060.416	–0.003	7.9830	b	209.31
24	14	11	24	13	12	628 107.093	–0.003	8.6553	b	216.07
25	14	12	25	13	13	628 154.764	0.011	9.3160	b	223.11
26	14	13	26	13	14	628 203.262	–0.009	9.9665	b	230.42
74	14	60	74	13	61	628 230.589	–0.050	38.6582	b	911.83
27	14	14	27	13	15	628 252.556	0.024	10.6081	b	238.02
28	14	15	28	13	16	628 302.392	–0.016	11.2419	b	245.91
29	14	16	29	13	17	628 352.776	0.005	11.8688	b	254.07
30	14	17	30	13	18	628 403.496	0.009	12.4896	b	262.51
32	14	19	32	13	20	628 505.411	–0.011	13.7158	b	280.24
74	5	69	73	5	68	628 510.845	0.002	73.5435	a	787.77
33	14	20	33	13	21	628 556.355	0.003	14.3223	b	289.53
71	14	57	71	13	58	628 585.121	–0.028	36.8196	b	850.34
34	14	21	34	13	22	628 607.048	–0.011	14.9252	b	299.10
35	14	22	35	13	23	628 657.403	0.017	15.5249	b	308.95
36	14	23	36	13	24	628 707.188	0.012	16.1217	b	319.08
37	14	24	37	13	25	628 756.266	0.001	16.7161	b	329.49
69	14	55	69	13	56	628 776.309	–0.005	35.6034	b	810.75
38	14	25	38	13	26	628 804.442	–0.046	17.3083	b	340.18
39	14	26	39	13	27	628 851.756	0.083	17.8987	b	351.15
68	14	54	68	13	55	628 859.272	–0.001	34.9981	b	791.37
40	14	27	40	13	28	628 897.642	–0.003	18.4876	b	362.41
67	14	54	67	13	55	628 934.180	–0.037	34.3944	b	772.27
41	14	28	41	13	29	628 942.236	0.010	19.0751	b	373.94
42	14	29	42	13	30	628 985.211	–0.022	19.6615	b	385.76
77	3	75	76	3	74	629 016.274	–0.037	76.7072	a	816.54
65	14	52	65	13	53	629 061.114	–0.119	33.1921	b	734.91
44	14	31	44	13	32	629 065.787	0.012	20.8320	b	410.23
45	14	32	45	13	33	629 102.950	0.025	21.4163	b	422.89
64	14	51	64	13	52	629 113.845	–0.034	32.5933	b	716.65
46	14	33	46	13	34	629 137.741	0.010	22.0004	b	435.83
47	14	34	47	13	35	629 170.018	0.028	22.5842	b	449.05
49	14	36	49	13	37	629 226.068	0.026	23.7519	b	476.33
61	14	48	61	13	49	629 231.721	0.004	30.8057	b	663.55
50	14	37	50	13	38	629 249.428	0.017	24.3360	b	490.39
60	14	47	60	13	48	629 258.527	–0.006	30.2126	b	646.40
51	14	38	51	13	39	629 269.434	0.049	24.9205	b	504.73
59	14	46	59	13	47	629 279.555	–0.003	29.6207	b	629.54
22	10	12	21	9	13	629 284.212	–0.049	11.0934	b	128.20
22	10	13	21	9	12	629 284.212	–0.049	11.0934	b	128.20
52	14	39	52	13	40	629 285.760	0.016	25.5054	b	519.35
58	14	45	58	13	46	629 295.074	0.023	29.0299	b	612.96
53	14	40	53	13	41	629 298.269	0.008	26.0909	b	534.25
57	14	43	57	13	44	629 305.246	–0.018	28.4402	b	596.66
54	14	41	54	13	42	629 306.753	0.046	26.6770	b	549.43
78	2	77	77	2	76	630 673.652	0.075	77.8158	a	823.08

Table 5. continued.

Transition						Obs. Freq.	obs.- calc.	S	Dipole	E_l
J'	K'_a	K'_c	J''	K''_a	K''_c	(MHz)	(MHz)			(cm^{-1})
78	1	77	77	1	76	630 673.652	–0.050	77.8158	a	823.08
75	16	60	74	16	59	630 945.011	–0.032	71.5894	a	979.40
75	15	61	74	15	60	630 947.454	0.007	72.0029	a	955.31
75	17	59	74	17	58	630 990.785	0.020	71.1492	a	1005.04
75	14	62	74	14	61	631 009.251	0.000	72.3898	a	932.78
75	18	58	74	18	57	631 076.581	0.016	70.6824	a	1032.21
75	6	70	74	6	69	631 083.508	0.017	74.4536	a	810.36
75	13	63	74	13	62	631 146.773	0.007	72.7501	a	911.83
75	13	62	74	13	61	631 146.773	0.003	72.7501	a	911.83
75	19	57	74	19	56	631 196.557	0.013	70.1889	a	1060.91
75	20	56	74	20	55	631 346.294	0.014	69.6687	a	1091.12
75	12	64	74	12	63	631 384.587	0.043	73.0838	a	892.47
75	12	63	74	12	62	631 384.587	–0.038	73.0838	a	892.47
75	21	55	74	21	54	631 522.405	0.011	69.1219	a	1122.84
75	22	54	74	22	53	631 722.282	0.027	68.5485	a	1156.05
74	7	67	73	7	66	631 755.465	–0.011	73.3729	a	801.21
75	11	65	74	11	64	631 761.127	–0.022	73.3909	a	874.73
75	11	64	74	11	63	631 762.599	0.012	73.3909	a	874.73
75	23	53	74	23	52	631 943.783	–0.002	67.9483	a	1190.74
75	24	52	74	24	51	632 185.333	0.017	67.3216	a	1226.91
75	10	66	74	10	65	632 336.096	0.013	73.6714	a	858.65
75	10	65	74	10	64	632 356.452	0.000	73.6714	a	858.66
79	1	79	78	1	78	632 371.594	0.012	78.9363	a	828.52
79	0	79	78	0	78	632 371.594	0.010	78.9363	a	828.52
75	25	51	74	25	50	632 445.528	0.037	66.6681	a	1264.54
75	26	50	74	26	49	632 723.192	–0.001	65.9880	a	1303.63
75	27	49	74	27	48	633 017.521	0.033	65.2812	a	1344.16
75	9	67	74	9	66	633 161.457	–0.009	73.9251	a	844.29
17	11	7	16	10	6	633 306.794	0.031	11.0454	b	116.27
17	11	6	16	10	7	633 306.794	0.031	11.0454	b	116.27
75	28	48	74	28	47	633 327.518	–0.068	64.5478	a	1386.13
75	9	66	74	9	65	633 381.795	–0.007	73.9256	a	844.32
28	9	20	27	8	19	633 395.890	–0.109	11.5006	b	156.31
76	5	72	75	5	71	633 745.475	0.015	75.5329	a	820.64
75	7	69	74	7	68	633 834.261	–0.007	74.3321	a	820.63
74	6	68	73	6	67	634 415.440	–0.029	73.5674	a	794.29
77	4	74	76	4	73	635 336.223	0.004	76.6122	a	829.74
77	3	74	76	3	73	635 415.536	0.018	76.6127	a	829.73
75	8	67	74	8	66	635 686.875	–0.024	74.1549	a	831.97
75	5	70	74	5	69	636 199.175	–0.017	74.5330	a	808.74
78	3	76	77	3	75	636 902.223	–0.001	77.7069	a	837.53
79	2	78	78	2	77	638 563.032	0.064	78.8158	a	844.11
79	1	78	78	1	77	638 563.032	–0.036	78.8158	a	844.11
76	16	61	75	16	60	639 281.092	–0.010	72.6344	a	1000.45
76	15	62	75	15	61	639 288.856	–0.011	73.0425	a	976.36
76	17	60	75	17	59	639 323.053	0.010	72.2000	a	1026.09
76	14	63	75	14	62	639 358.079	–0.018	73.4243	a	953.83
76	18	59	75	18	58	639 406.320	0.014	71.7393	a	1053.26
76	13	64	75	13	63	639 505.830	–0.003	73.7799	a	932.88
76	13	63	75	13	62	639 505.830	–0.008	73.7799	a	932.88
76	19	58	75	19	57	639 524.752	–0.002	71.2523	a	1081.97
76	20	57	75	20	56	639 673.757	–0.031	70.7390	a	1112.18
76	12	65	75	12	64	639 757.808	0.017	74.1092	a	913.53
76	12	64	75	12	63	639 757.808	–0.091	74.1092	a	913.53
76	21	56	75	21	55	639 849.889	–0.007	70.1994	a	1143.90
76	22	55	75	22	54	640 050.348	0.002	69.6334	a	1177.12
76	11	66	75	11	65	640 154.402	–0.001	74.4123	a	895.80
76	11	65	75	11	64	640 156.256	–0.010	74.4123	a	895.80
80	1	80	79	1	79	640 262.605	0.010	79.9363	a	849.61
80	0	80	79	0	79	640 262.605	0.009	79.9363	a	849.61
76	23	54	75	23	53	640 272.990	0.011	69.0412	a	1211.82
75	7	68	74	7	67	640 636.381	–0.049	74.3877	a	822.28
76	25	52	75	25	51	640 778.188	–0.012	67.7778	a	1285.64
76	10	66	75	10	65	640 782.792	–0.021	74.6892	a	879.75
76	9	68	75	9	67	641 611.682	–0.025	74.9396	a	865.41
77	5	73	76	5	72	641 649.704	0.005	76.5318	a	841.78

Table 5. continued.

Transition						Obs. Freq.	obs.- calc.	S	Dipole	E_l
J'	K'_a	K'_c	J''	K''_a	K''_c	(MHz)	(MHz)			(cm^{-1})
29	9	21	28	8	20	641 806.039	–0.080	11.6925	b	164.19
29	9	20	28	8	21	641 806.039	–0.083	11.6925	b	164.19
76	7	70	75	7	69	642 114.324	–0.009	75.3380	a	841.77
76	8	69	75	8	68	642 454.900	–0.035	75.1607	a	852.83
77	4	73	76	4	72	642 463.583	–0.024	76.5376	a	841.60

Table 6. Measured transitions of the ground vibrational state of CH_2DCH_2CN out-of-plane.

Transition						Obs. Freq.	obs.- calc.	S	Dipole	E_l
J'	K'_a	K'_c	J''	K''_a	K''_c	(MHz)	(MHz)			(cm^{-1})
22	4	18	21	5	17	8505.160	–0.007	3.3575	b	84.32
6	2	4	7	1	7	8520.324	0.006	0.8664	b	8.58
1	0	1	0	0	0	8693.720	0.004	1.0000	a	0.00
29	4	25	29	4	26	8713.615	0.001	0.9523	a	137.58
10	1	10	9	2	7	8777.717	–0.014	1.1077	b	15.88
38	5	33	38	5	34	8862.059	0.000	1.1166	a	232.89
38	9	30	39	8	31	9150.310	0.088	5.8015	b	270.62
10	3	7	11	2	10	9258.390	–0.006	1.5568	b	21.87
6	1	5	6	1	6	9927.536	0.018	0.3104	a	6.61
13	2	11	13	2	12	9979.460	0.036	0.5423	a	29.09
21	3	18	21	3	19	9984.452	0.021	0.7427	a	73.33
19	5	15	20	4	16	9985.854	–0.039	2.9272	b	72.07
27	5	23	26	6	20	10 265.926	0.001	4.1274	b	126.75
19	5	14	20	4	17	10 539.037	–0.016	2.9244	b	72.05
27	5	22	26	6	21	10 644.847	–0.027	4.1292	b	126.75
30	4	26	30	4	27	11 042.694	–0.011	0.9021	a	146.32
39	5	34	39	5	35	11 094.789	–0.011	1.0672	a	244.26
33	8	26	34	7	27	11 610.053	0.074	5.0293	b	206.59
33	8	25	34	7	28	11 621.005	0.054	5.0292	b	206.59
14	4	11	15	3	12	12 058.793	–0.032	2.1552	b	41.11
18	3	16	17	4	13	12 382.174	–0.003	2.7638	b	55.48
22	3	19	22	3	20	12 721.742	–0.002	0.6935	a	79.72
32	6	27	31	7	24	12 898.634	–0.053	4.9010	b	177.81
14	2	12	14	2	13	12 930.827	0.052	0.4944	a	33.13
32	6	26	31	7	25	13 016.012	–0.051	4.9014	b	177.81
7	1	6	7	1	7	13 227.117	0.027	0.2693	a	8.58
11	1	11	10	2	8	13 439.551	–0.039	1.1165	b	18.82
9	3	7	10	2	8	13 519.020	–0.045	1.3915	b	18.82
14	4	10	15	3	13	13 640.468	–0.025	2.1449	b	41.06
40	5	35	40	5	36	13 754.633	–0.010	1.0186	a	255.93
31	4	27	31	4	28	13 820.718	–0.018	0.8536	a	155.35
28	7	22	29	6	23	14 115.276	–0.014	4.2564	b	151.18
28	7	21	29	6	24	14 152.262	–0.007	4.2563	b	151.18
14	2	13	13	3	10	14 172.439	0.002	2.0809	b	32.66
4	2	3	5	1	4	15 060.282	0.002	0.6499	b	5.16
5	2	3	6	1	6	15 209.902	0.020	0.7182	b	6.61
4	0	4	3	1	3	15 400.948	0.029	1.6290	b	2.38
8	1	7	7	2	6	15 742.581	0.064	1.5361	b	10.87
23	3	20	23	3	21	15 947.741	0.000	0.6477	a	86.39
23	4	20	22	5	17	16 299.113	0.032	3.5581	b	90.72
15	2	13	15	2	14	16 371.830	0.052	0.4527	a	37.45
23	6	18	24	5	19	16 632.881	–0.048	3.4829	b	104.40
23	6	17	24	5	20	16 752.974	–0.045	3.4825	b	104.39
18	3	15	17	4	14	16 865.617	0.051	2.8063	b	55.47
2	1	2	1	1	1	16 914.335	0.001	1.5000	a	0.97
8	1	7	8	1	8	16 988.077	0.043	0.2383	a	10.83
13	2	11	12	3	10	16 998.902	0.054	2.0936	b	28.86
2	0	2	1	0	1	17 379.240	0.004	1.9998	a	0.29
1	1	0	1	0	1	20 912.340	0.022	1.5000	b	0.29
2	1	1	2	0	2	21 393.790	0.010	2.4712	b	0.87
3	1	2	3	0	3	22 131.110	0.015	3.3993	b	1.74
3	1	3	2	1	2	25 366.350	0.025	2.6666	a	1.54
3	0	3	2	0	2	26 048.440	0.055	2.9992	a	0.87
3	2	2	2	2	1	26 081.880	0.075	1.6667	a	3.63
3	2	1	2	2	0	26 114.200	–0.066	1.6667	a	3.63
3	1	2	2	1	1	26 785.620	–0.081	2.6666	a	1.58
1	1	1	0	0	0	29 132.850	0.016	1.0000	b	0.00
2	1	2	1	0	1	37 353.490	0.038	1.5000	b	0.29
17	1	17	16	1	16	142 528.858	0.049	16.9243	a	38.88
18	0	18	17	1	17	148 133.398	0.023	14.1279	b	43.64
17	1	16	16	1	15	149 632.173	0.100	16.8969	a	40.95
18	1	18	17	1	17	150 801.915	0.067	17.9257	a	43.64
28	4	25	28	3	26	151 323.292	–0.020	15.4325	b	124.08
18	0	18	17	0	17	151 404.189	0.023	17.9365	a	43.53
48	4	44	48	3	45	154 670.839	0.007	29.8448	b	351.99

Table 6. continued.

Transition						Obs. Freq.	obs.- calc.	S	Dipole	E_l
J'	K'_a	K'_c	J''	K''_a	K''_c	(MHz)	(MHz)			(cm^{-1})
55	6	49	55	5	50	155 483.536	0.012	41.9160	b	469.31
19	2	18	18	2	17	163 656.895	0.006	18.7673	a	52.13
19	9	10	18	9	9	165 358.924	0.088	14.7373	a	105.41
19	11	8	18	11	7	165 380.203	0.022	12.6320	a	132.90
19	7	13	18	7	12	165 387.922	0.035	16.4215	a	83.39
19	7	12	18	7	11	165 387.922	0.033	16.4215	a	83.39
19	12	7	18	12	6	165 402.146	0.013	11.4214	a	148.69
19	13	6	18	13	5	165 429.794	0.013	10.1056	a	165.83
19	6	14	18	6	13	165 440.110	0.079	17.1057	a	74.45
19	6	13	18	6	12	165 440.110	–0.035	17.1057	a	74.45
19	5	15	18	5	14	165 543.320	0.039	17.6845	a	66.88
19	5	14	18	5	13	165 548.205	0.003	17.6845	a	66.88
19	3	17	18	3	16	165 566.094	0.024	18.5216	a	55.89
19	4	16	18	4	15	165 708.588	0.052	18.1575	a	60.71
19	4	15	18	4	14	165 833.385	0.010	18.1575	a	60.71
19	1	18	18	1	17	166 510.726	0.044	18.8835	a	51.22
19	3	16	18	3	15	167 067.988	0.004	18.5252	a	56.03
20	1	20	19	1	19	167 319.526	0.030	19.9274	a	53.97
20	0	20	19	0	19	167 738.256	0.052	19.9335	a	53.90
19	2	17	18	2	16	169 057.543	0.064	18.7987	a	53.12
20	9	12	19	9	11	174 065.366	0.033	15.9505	a	110.93
20	10	11	19	10	10	174 069.457	0.020	15.0005	a	123.99
20	8	13	19	8	12	174 074.868	0.020	16.8005	a	99.23
20	11	10	19	11	9	174 083.423	–0.023	13.9505	a	138.42
20	13	8	19	13	7	174 133.208	0.044	11.5504	a	171.35
20	14	6	19	14	5	174 166.584	0.007	10.2003	a	189.85
20	6	14	19	6	13	174 167.838	–0.058	18.2004	a	79.97
20	15	6	19	15	5	174 204.765	–0.006	8.7503	a	209.70
20	3	18	19	3	17	174 251.050	0.049	19.5440	a	61.41
20	5	16	19	5	15	174 289.302	0.011	18.7502	a	72.40
20	5	15	19	5	14	174 297.109	–0.009	18.7502	a	72.41
16	2	15	15	1	14	174 413.863	0.022	6.3153	b	36.25
20	4	16	19	4	15	174 648.267	0.088	19.1995	a	66.25
20	1	19	19	1	18	174 861.548	0.048	19.8754	a	56.77
21	1	21	20	1	20	175 566.082	0.057	20.9280	a	59.55
21	0	21	20	0	20	175 910.461	0.010	20.9326	a	59.50
20	3	17	19	3	16	176 120.441	0.020	19.5497	a	61.61
21	1	21	20	0	20	177 311.132	0.020	17.2755	b	59.50
20	2	18	19	2	17	177 965.421	0.021	19.8080	a	58.76
27	5	22	27	4	23	178 625.854	–0.024	14.9558	b	121.15
38	4	35	38	3	36	178 861.263	0.026	19.0072	b	220.65
22	0	22	21	1	21	182 686.166	0.024	18.2760	b	65.41
21	9	13	20	9	12	182 772.373	0.037	17.1434	a	116.73
21	10	12	20	10	11	182 773.915	0.035	16.2386	a	129.79
21	12	10	20	12	9	182 807.831	0.033	14.1433	a	160.01
21	7	14	20	7	13	182 823.264	–0.007	18.6672	a	94.72
21	7	15	20	7	14	182 823.264	0.000	18.6672	a	94.72
23	1	22	22	2	21	182 832.163	–0.003	11.3730	b	75.66
21	14	8	20	14	7	182 870.150	0.011	11.6670	a	195.66
21	15	7	20	15	6	182 909.520	0.048	10.2860	a	215.51
21	3	19	20	3	18	182 921.801	0.019	20.5639	a	67.22
21	16	6	20	16	5	182 953.500	–0.006	8.8098	a	236.71
21	5	17	20	5	16	183 040.065	0.024	19.8097	a	78.22
21	5	16	20	5	15	183 052.204	0.015	19.8097	a	78.22
21	1	20	20	1	19	183 156.491	0.028	20.8668	a	62.60
21	4	18	20	4	17	183 235.279	0.045	20.2373	a	72.05
29	5	25	29	4	26	183 324.143	0.007	16.1220	b	137.58
22	5	17	22	4	18	183 340.741	0.024	11.6690	b	84.61
30	5	26	30	4	27	183 349.101	0.013	16.7711	b	146.32
28	5	24	28	4	25	183 371.270	0.029	15.4730	b	129.13
27	5	23	27	4	24	183 475.472	0.042	14.8256	b	120.98
21	4	17	20	4	16	183 482.250	0.051	20.2374	a	72.07
26	5	22	26	4	23	183 622.883	0.017	14.1812	b	113.11
47	6	41	47	5	42	183 663.482	–0.046	30.1738	b	347.25
32	5	28	32	4	29	183 679.458	0.019	18.0612	b	164.66
25	5	21	25	4	22	183 801.037	0.018	13.5407	b	105.54

Table 6. continued.

Transition						Obs. Freq.	obs.- calc.	S	Dipole	E_l
J'	K'_a	K'_c	J''	K''_a	K''_c	(MHz)	(MHz)			(cm^{-1})
22	1	22	21	1	21	183 805.585	0.016	21.9283	a	65.41
24	5	20	24	4	21	183 998.807	0.021	12.9050	b	98.26
33	5	29	33	4	30	184 018.409	0.013	18.6975	b	174.27
38	2	36	38	1	37	184 050.879	–0.018	13.3909	b	214.15
22	0	22	21	0	21	184 086.807	0.004	21.9318	a	65.36
23	5	19	23	4	20	184 206.554	–0.004	12.2744	b	91.27
20	5	15	20	4	16	184 294.894	0.003	10.4236	b	72.07
22	5	18	22	4	19	184 416.268	0.018	11.6493	b	84.57
34	5	30	34	4	31	184 495.975	0.021	19.3245	b	184.17
21	5	17	21	4	18	184 621.271	–0.001	11.0296	b	78.17
19	5	14	19	4	15	184 645.975	0.023	9.8112	b	66.25
20	5	16	20	4	17	184 816.474	0.010	10.4153	b	72.05
33	1	32	33	0	33	184 881.305	0.072	6.6444	b	157.08
18	5	13	18	4	14	184 931.148	0.024	9.2043	b	60.71
19	5	15	19	4	16	184 997.996	–0.003	9.8059	b	66.23
35	5	31	35	4	32	185 128.989	–0.016	19.9392	b	194.35
17	5	12	17	4	13	185 161.534	0.028	8.6021	b	55.48
18	5	14	18	4	15	185 163.272	0.018	9.2011	b	60.71
21	3	18	20	3	17	185 204.626	0.027	20.5725	a	67.48
22	1	22	21	0	21	185 206.240	0.010	18.2990	b	65.36
17	5	13	17	4	14	185 310.689	0.024	8.6001	b	55.47
16	5	12	16	4	13	185 439.572	–0.006	8.0022	b	50.53
15	5	10	15	4	11	185 493.786	0.005	7.4069	b	45.88
18	2	17	17	1	16	185 558.635	0.006	7.5953	b	45.94
14	5	9	14	4	10	185 610.074	0.017	6.8115	b	41.52
14	5	10	14	4	11	185 642.960	0.090	6.8112	b	41.52
13	5	9	13	4	10	185 719.028	–0.050	6.2153	b	37.45
12	5	8	12	4	9	185 780.191	0.023	5.6166	b	33.67
36	5	32	36	4	33	185 933.927	–0.013	20.5386	b	204.82
22	1	21	21	1	20	191 400.724	0.056	21.8580	a	68.71
23	1	23	22	1	22	192 038.951	–0.004	22.9286	a	71.54
23	0	23	22	0	22	192 267.161	0.043	22.9312	a	71.50
23	2	22	22	2	21	197 330.242	0.023	22.7894	a	75.66
23	1	22	22	1	21	199 601.120	0.024	22.8495	a	75.10
44	5	40	44	4	41	200 150.336	–0.037	24.4636	b	298.80
23	10	14	22	10	13	200 183.163	0.011	18.6528	a	142.28
23	9	15	22	9	14	200 187.961	0.009	19.4789	a	129.22
23	11	13	22	11	12	200 192.255	0.003	17.7397	a	156.71
23	3	21	22	3	20	200 213.919	0.030	22.5973	a	79.72
23	13	11	22	13	10	200 239.957	–0.016	15.6527	a	189.65
23	14	10	22	14	9	200 275.102	–0.013	14.4787	a	208.15
23	15	9	22	15	8	200 316.428	0.042	13.2178	a	228.01
23	16	8	22	16	7	200 363.098	–0.032	11.8699	a	249.21
23	6	18	22	6	17	200 369.921	–0.004	21.4353	a	98.27
23	6	17	22	6	16	200 370.868	–0.019	21.4353	a	98.27
23	17	7	22	17	6	200 414.871	–0.006	10.4351	a	271.75
24	0	24	23	0	23	200 450.999	–0.003	23.9308	a	77.92
23	5	19	22	5	18	200 555.950	0.017	21.9132	a	90.72
23	5	18	22	5	17	200 583.328	–0.028	21.9132	a	90.72
23	4	20	22	4	19	200 765.597	–0.028	22.3029	a	84.57
28	2	26	27	3	25	201 109.133	–0.022	8.6888	b	115.98
24	1	24	23	0	23	201 158.187	–0.009	20.3402	b	77.92
23	4	19	22	4	18	201 219.120	–0.005	22.3033	a	84.61
42	6	36	42	5	37	202 607.143	0.029	24.9603	b	280.81
45	5	41	45	4	42	203 030.308	–0.047	24.8177	b	311.82
23	3	20	22	3	19	203 439.898	0.011	22.6142	a	80.14
25	1	24	24	2	23	203 474.049	0.015	13.4743	b	89.10
23	2	21	22	2	20	204 412.807	0.013	22.8227	a	77.46
24	1	23	23	1	22	207 765.974	–0.042	23.8417	a	81.76
25	0	25	24	1	24	207 930.743	0.006	21.3481	b	84.63
22	2	21	21	1	20	208 169.578	–0.020	10.8238	b	68.71
40	6	34	40	5	35	208 426.395	0.011	23.2737	b	256.39
25	0	25	24	0	24	208 637.929	–0.003	24.9304	a	84.60
24	3	22	23	3	21	208 832.076	0.004	23.6112	a	86.39
24	10	15	23	10	14	208 887.975	–0.010	19.8340	a	148.96

Table 6. continued.

J'	K_a'	K_c'	J''	K_a''	K_c''	Obs. Freq. (MHz)	obs.- calc. (MHz)	S	Dipole	E_l (cm^{-1})
24	11	14	23	11	13	208 894.805	–0.016	18.9590	a	163.39
24	9	16	23	9	15	208 896.597	–0.011	20.6257	a	135.89
24	12	13	23	12	12	208 913.294	–0.006	18.0006	a	179.18
24	8	17	23	8	16	208 927.129	0.004	21.3340	a	124.20
24	13	12	23	13	11	208 941.021	–0.012	16.9589	a	196.33
24	14	11	23	14	10	208 976.443	–0.016	15.8339	a	214.83
24	7	17	23	7	16	208 991.148	–0.025	21.9589	a	113.89
24	7	18	23	7	17	208 991.148	0.013	21.9589	a	113.89
24	15	10	23	15	9	209 018.496	–0.023	14.6255	a	234.69
24	16	9	23	16	8	209 066.456	–0.015	13.3338	a	255.89
24	6	19	23	6	18	209 110.898	–0.009	22.5005	a	104.95
24	6	18	23	6	17	209 112.431	–0.018	22.5005	a	104.95
24	5	20	23	5	19	209 320.973	–0.013	22.9584	a	97.41
24	5	19	23	5	18	209 361.034	0.018	22.9584	a	97.41
24	4	21	23	4	20	209 528.750	–0.009	23.3315	a	91.27
24	4	20	23	4	19	210 128.077	0.024	23.3321	a	91.32
39	6	33	39	5	34	210 903.066	–0.004	22.4826	b	244.63
25	1	24	24	1	23	215 904.186	–0.037	24.8346	a	88.69
26	1	26	25	1	25	216 709.260	0.030	25.9290	a	91.58
26	0	26	25	0	25	216 827.371	0.029	25.9301	a	91.56
39	6	34	39	5	35	220 895.121	0.027	22.1752	b	244.26
44	6	39	44	5	40	221 000.246	0.022	25.5516	b	305.48
45	6	40	45	5	41	221 403.570	0.022	26.2021	b	318.59
37	6	32	37	5	33	221 442.641	–0.036	20.8092	b	221.81
32	6	26	32	5	27	221 580.826	0.008	17.4900	b	170.85
25	3	22	24	3	21	221 701.029	0.013	24.6520	a	94.02
25	2	23	24	2	22	221 775.867	–0.028	24.8219	a	91.38
36	6	31	36	5	32	221 783.590	0.004	20.1298	b	211.02
49	3	46	49	2	47	221 905.532	0.019	20.2896	b	358.79
46	6	41	46	5	42	221 972.767	–0.026	26.8382	b	331.99
26	2	25	25	2	24	222 378.448	0.002	25.7972	a	96.24
30	6	24	30	5	25	223 124.915	0.049	16.1720	b	152.47
27	1	26	26	2	25	223 206.302	–0.030	15.6299	b	103.66
32	6	27	32	5	28	223 325.004	0.036	17.4578	b	170.79
48	6	43	48	5	44	223 670.889	0.008	28.0555	b	359.64
31	6	26	31	5	27	223 710.153	–0.049	16.8040	b	161.47
29	6	23	29	5	24	223 740.591	0.028	15.5256	b	143.72
43	3	41	43	2	42	223 877.433	–0.001	13.3561	b	271.88
26	1	25	25	1	24	224 024.233	–0.021	25.8285	a	95.89
30	6	25	30	5	26	224 082.227	–0.002	16.1563	b	152.43
28	6	22	28	5	23	224 270.732	–0.038	14.8866	b	135.27
29	6	24	29	5	25	224 436.659	0.008	15.5147	b	143.70
27	0	27	26	1	26	224 577.317	–0.043	23.3825	b	98.81
27	6	21	27	5	22	224 727.225	0.005	14.2545	b	127.11
28	6	23	28	5	24	224 770.104	–0.072	14.8792	b	135.25
27	1	27	26	1	26	224 924.597	–0.033	26.9290	a	98.81
15	3	13	14	2	12	224 937.468	0.027	4.5991	b	33.56
27	0	27	26	0	26	225 018.660	–0.014	26.9298	a	98.80
27	6	22	27	5	23	225 080.515	0.013	14.2495	b	127.10
26	6	20	26	5	21	225 120.022	0.029	13.6288	b	119.24
25	6	19	25	5	20	225 457.701	–0.010	13.0089	b	111.67
25	6	20	25	5	21	225 626.594	0.015	13.0068	b	111.67
24	6	18	24	5	19	225 747.708	–0.013	12.3943	b	104.40
24	6	19	24	5	20	225 861.555	–0.028	12.3929	b	104.39
23	6	17	23	5	18	225 996.301	0.014	11.7845	b	97.41
26	3	24	25	3	23	226 006.141	–0.005	25.6344	a	100.61
23	6	18	23	5	19	226 071.609	–0.053	11.7836	b	97.41
26	10	16	25	10	15	226 298.040	–0.017	22.1546	a	163.18
26	11	15	25	11	14	226 299.334	–0.010	21.3469	a	177.61
26	9	17	25	9	16	226 315.629	–0.091	22.8853	a	150.12
26	13	13	25	13	12	226 341.161	–0.003	19.5006	a	210.56
26	8	19	25	8	18	226 360.507	–0.032	23.5392	a	138.43
26	8	18	25	8	17	226 360.507	–0.034	23.5392	a	138.43
26	14	12	25	14	11	226 376.644	–0.038	18.4621	a	229.07
26	15	11	25	15	10	226 419.853	–0.084	17.3467	a	248.92
26	7	20	25	7	19	226 447.359	0.030	24.1160	a	128.12

Table 6. continued.

Transition						Obs. Freq.	obs.- calc.	S	Dipole	E_l
J'	K'_a	K'_c	J''	K''_a	K''_c	(MHz)	(MHz)			(cm^{-1})
26	7	19	25	7	18	226 447.359	–0.081	24.1160	a	128.12
26	6	21	25	6	20	226 604.034	–0.017	24.6159	a	119.19
26	6	20	25	6	19	226 607.781	0.010	24.6159	a	119.19
26	5	22	25	5	21	226 864.385	–0.046	25.0384	a	111.67
26	5	21	25	5	20	226 945.488	0.000	25.0384	a	111.67
26	4	23	25	4	22	227 042.567	–0.018	25.3816	a	105.54
26	2	24	25	2	23	230 366.499	–0.024	25.8185	a	98.78
26	3	23	25	3	22	230 815.001	0.015	25.6693	a	101.41
28	1	28	27	1	27	233 136.779	–0.007	27.9290	a	106.31
28	0	28	27	0	27	233 211.372	–0.036	27.9296	a	106.30
27	11	17	26	11	16	235 001.250	–0.024	22.5193	a	185.16
27	10	18	26	10	17	235 003.275	–0.025	23.2971	a	170.73
27	12	16	26	12	15	235 014.661	–0.037	21.6674	a	200.95
27	9	19	26	9	18	235 026.176	–0.043	24.0008	a	157.67
27	13	15	26	13	14	235 040.114	–0.062	20.7414	a	218.11
27	8	20	26	8	19	235 079.233	–0.004	24.6304	a	145.98
27	8	19	26	8	18	235 079.233	–0.008	24.6304	a	145.98
28	2	27	27	2	26	238 991.357	–0.076	27.7998	a	111.35
28	1	27	27	1	26	240 238.941	–0.040	27.8191	a	111.10
28	11	17	27	11	16	243 702.950	–0.016	23.6794	a	193.00
28	8	21	27	8	20	243 799.325	–0.006	25.7151	a	153.82
28	8	20	27	8	19	243 799.325	–0.013	25.7151	a	153.82
28	7	22	27	7	21	243 913.271	0.114	26.2507	a	143.52
28	6	23	27	6	22	244 112.916	0.055	26.7148	a	134.60
28	6	22	27	6	21	244 121.183	–0.037	26.7148	a	134.60
28	5	24	27	5	23	244 423.079	–0.109	27.1069	a	127.10
28	4	25	27	4	24	244 527.299	–0.077	27.4238	a	120.98
28	5	23	27	5	22	244 577.683	0.014	27.1070	a	127.11
28	4	24	27	4	23	246 096.865	–0.093	27.4278	a	121.15
28	2	26	27	2	25	247 353.324	0.026	27.8062	a	114.43
28	3	25	27	3	24	248 960.772	–0.075	27.6995	a	117.11
67	18	50	66	18	49	581 757.146	–0.007	62.1673	a	863.83
67	15	53	66	15	52	581 767.715	0.021	63.6454	a	796.00
67	19	49	66	19	48	581 826.168	0.000	61.6149	a	889.16
67	14	54	66	14	53	581 872.074	–0.020	64.0785	a	776.14
67	20	48	66	20	47	581 922.602	–0.002	61.0326	a	915.83
67	6	62	66	6	61	582 016.681	–0.029	66.3847	a	668.29
67	21	47	66	21	46	582 043.028	–0.008	60.4206	a	943.83
67	13	55	66	13	54	582 050.638	–0.002	64.4818	a	757.67
67	13	54	66	13	53	582 050.638	–0.006	64.4818	a	757.67
67	22	46	66	22	45	582 184.782	–0.020	59.7786	a	973.17
67	12	56	66	12	55	582 328.371	0.012	64.8552	a	740.61
67	12	55	66	12	54	582 328.371	–0.080	64.8552	a	740.61
70	2	69	69	2	68	582 330.386	–0.033	69.7924	a	681.64
67	23	45	66	23	44	582 345.796	–0.006	59.1069	a	1003.82
67	24	44	66	24	43	582 524.381	0.026	58.4053	a	1035.79
66	7	59	65	7	58	582 691.375	0.028	65.2984	a	659.47
67	25	43	66	25	42	582 719.132	0.035	57.6738	a	1069.06
67	11	57	66	11	56	582 744.491	–0.100	65.1989	a	724.99
67	11	56	66	11	55	582 746.208	0.009	65.1989	a	724.99
67	26	42	66	26	41	582 928.887	–0.019	56.9125	a	1103.64
67	27	41	66	27	40	583 152.842	–0.008	56.1214	a	1139.50
67	10	58	66	10	57	583 359.724	0.037	65.5129	a	710.83
67	10	57	66	10	56	583 382.246	–0.001	65.5129	a	710.84
67	28	40	66	28	39	583 390.131	–0.014	55.3004	a	1176.65
67	29	39	66	29	38	583 640.125	0.002	54.4495	a	1215.07
67	30	38	66	30	37	583 902.206	–0.006	53.5688	a	1254.76
67	31	37	66	31	36	584 175.914	0.002	52.6583	a	1295.71
67	9	59	66	9	58	584 222.814	0.012	65.7968	a	698.20
67	9	58	66	9	57	584 463.798	0.045	65.7973	a	698.23
67	7	61	66	7	60	584 856.446	–0.034	66.2505	a	677.37
68	5	64	67	5	63	584 859.516	–0.009	67.4728	a	678.14
67	8	60	66	8	59	585 097.698	–0.019	66.0478	a	687.10
66	6	60	65	6	59	585 163.024	–0.003	65.5123	a	653.40
27	9	19	26	8	18	585 418.161	–0.085	11.2126	b	145.98
27	9	18	26	8	19	585 418.161	–0.090	11.2126	b	145.98

Table 6. continued.

Transition						Obs. Freq.	obs.- calc.	S	Dipole	E_l
J'	K'_a	K'_c	J''	K''_a	K''_c	(MHz)	(MHz)			(cm^{-1})
68	4	64	67	4	63	585 716.582	–0.034	67.4796	a	677.96
69	4	66	68	4	65	586 689.334	0.006	68.5624	a	686.91
69	3	66	68	3	65	586 758.159	0.005	68.5628	a	686.90
67	8	59	66	8	58	586 882.878	0.037	66.0541	a	687.37
67	5	62	66	5	61	586 929.418	–0.063	66.4674	a	666.93
70	3	68	69	3	67	588 517.311	–0.008	69.6695	a	694.52
70	2	68	69	2	67	588 520.464	–0.003	69.6695	a	694.52
18	11	8	17	10	7	589 181.422	–0.012	11.1686	b	113.25
18	11	7	17	10	8	589 181.422	–0.012	11.1686	b	113.25
68	6	63	67	6	62	590 302.417	–0.015	67.3854	a	687.70
68	17	52	67	17	51	590 329.076	0.012	63.7534	a	859.26
68	16	53	67	16	52	590 334.835	0.005	64.2389	a	836.65
68	18	51	67	18	50	590 362.588	0.003	63.2385	a	883.24
68	15	54	67	15	53	590 388.453	0.006	64.6950	a	815.41
68	19	50	67	19	49	590 429.134	0.005	62.6942	a	908.57
71	2	70	70	2	69	590 443.311	–0.027	70.7924	a	701.07
71	1	70	70	1	69	590 443.311	–0.107	70.7924	a	701.07
68	14	55	67	14	54	590 501.948	0.009	65.1217	a	795.55
68	20	49	67	20	48	590 524.012	0.005	62.1205	a	935.24
68	21	48	67	21	47	590 643.635	–0.008	61.5174	a	963.25
68	13	56	67	13	55	590 692.780	0.023	65.5190	a	777.09
68	22	47	67	22	46	590 785.258	–0.001	60.8850	a	992.59
68	23	46	67	23	45	590 946.692	0.029	60.2231	a	1023.25
68	12	57	67	12	56	590 987.344	0.070	65.8871	a	760.04
68	12	56	67	12	55	590 987.344	–0.056	65.8871	a	760.04
68	24	45	67	24	44	591 126.115	0.013	59.5318	a	1055.22
68	25	44	67	25	43	591 322.161	0.006	58.8111	a	1088.50
68	11	58	67	11	57	591 426.980	–0.003	66.2258	a	744.43
68	11	57	67	11	56	591 429.136	0.001	66.2258	a	744.43
68	26	43	67	26	42	591 533.674	0.019	58.0610	a	1123.08
68	27	42	67	27	41	591 759.640	0.011	57.2814	a	1158.95
23	10	13	22	9	14	591 794.399	–0.085	11.2235	b	129.22
67	7	60	66	7	59	591 918.946	0.040	66.3172	a	678.91
68	28	41	67	28	40	591 999.278	0.015	56.4725	a	1196.11
68	10	59	67	10	58	592 074.466	0.021	66.5351	a	730.29
68	10	58	67	10	57	592 103.637	0.009	66.5352	a	730.30
68	9	60	67	9	59	592 970.239	0.014	66.8149	a	717.68
69	5	65	68	5	64	592 985.326	0.029	68.4713	a	697.65
68	9	59	67	9	58	593 270.447	0.036	66.8155	a	717.72
68	7	62	67	7	61	593 399.949	0.005	67.2577	a	696.88
69	4	65	68	4	64	593 709.797	–0.002	68.4769	a	697.50
67	6	61	66	6	60	593 733.846	–0.017	66.5116	a	672.92
68	8	61	67	8	60	593 819.022	0.002	67.0614	a	706.62
28	9	20	27	8	19	594 076.268	–0.109	11.3955	b	153.82
68	5	63	67	5	62	594 778.487	–0.047	67.4553	a	686.51
70	4	67	69	4	66	594 790.387	0.030	69.5615	a	706.48
70	3	67	69	3	66	594 846.478	0.029	69.5618	a	706.47
16	15	1	16	14	2	594 988.033	0.004	1.9035	b	174.17
70	15	55	70	14	56	594 998.899	0.036	36.2480	b	855.50
17	15	3	17	14	4	595 022.247	0.059	2.7799	b	179.11
18	15	3	18	14	4	595 057.803	0.012	3.6172	b	184.33
19	15	5	19	14	6	595 094.759	0.019	4.4216	b	189.85
14	12	2	13	11	3	595 107.938	–0.002	11.5765	b	109.67
14	12	3	13	11	2	595 107.938	–0.002	11.5765	b	109.67
20	15	6	20	14	7	595 132.984	0.050	5.1980	b	195.66
21	15	7	21	14	8	595 172.303	0.037	5.9505	b	201.76
24	15	10	24	14	11	595 295.986	0.029	8.0954	b	221.80
25	15	11	25	14	12	595 338.674	–0.006	8.7807	b	229.07
67	15	53	67	14	54	595 367.963	0.016	34.3976	b	795.55
26	15	12	26	14	13	595 381.949	0.015	9.4541	b	236.62
27	15	13	27	14	14	595 425.581	–0.004	10.1173	b	244.46
28	15	14	28	14	15	595 469.514	0.025	10.7713	b	252.59
66	15	52	66	14	53	595 472.421	0.073	33.7845	b	776.14
29	15	15	29	14	16	595 513.499	–0.004	11.4173	b	261.01
30	15	16	30	14	17	595 557.455	–0.020	12.0562	b	269.72
65	15	51	65	14	52	595 568.011	0.029	33.1731	b	757.02

Table 6. continued.

Transition						Obs. Freq.	obs.- calc.	S	Dipole	E_l
J'	K_a'	K_c'	J''	K_a''	K_c''	(MHz)	(MHz)			(cm^{-1})
31	15	17	31	14	18	595 601.268	0.018	12.6888	b	278.72
33	8	25	32	7	26	595 621.682	–0.075	11.5080	b	187.11
32	15	18	32	14	19	595 644.682	0.013	13.3159	b	288.02
64	15	50	64	14	51	595 655.185	0.013	32.5634	b	738.19
33	15	19	33	14	20	595 687.560	–0.007	13.9381	b	297.60
34	15	20	34	14	21	595 729.769	–0.006	14.5560	b	307.47
63	15	49	63	14	50	595 734.256	0.027	31.9553	b	719.64
35	15	21	35	14	22	595 771.096	–0.023	15.1701	b	317.63
62	15	48	62	14	49	595 805.463	–0.003	31.3486	b	701.38
36	15	22	36	14	23	595 811.414	–0.008	15.7808	b	328.08
37	15	23	37	14	24	595 850.494	–0.006	16.3886	b	338.82
61	15	47	61	14	48	595 869.196	0.012	30.7435	b	683.41
39	15	25	39	14	26	595 924.196	–0.035	17.5970	b	361.17
60	15	46	60	14	47	595 925.732	0.049	30.1397	b	665.73
68	8	60	67	8	59	595 934.997	0.041	67.0696	a	706.95
40	15	26	40	14	27	595 958.486	–0.010	18.1981	b	372.78
59	15	45	59	14	46	595 975.263	0.005	29.5372	b	648.34
41	15	27	41	14	28	595 990.736	–0.026	18.7977	b	384.68
58	15	44	58	14	45	596 018.201	0.004	28.9359	b	631.24
42	15	28	42	14	29	596 020.842	0.018	19.3959	b	396.87
43	15	29	43	14	30	596 048.457	–0.016	19.9930	b	409.35
57	15	43	57	14	44	596 054.842	0.057	28.3358	b	614.42
44	15	30	44	14	31	596 073.459	–0.036	20.5892	b	422.12
56	15	42	56	14	43	596 085.311	0.009	27.7367	b	597.90
45	15	31	45	14	32	596 095.657	–0.016	21.1848	b	435.18
55	15	41	55	14	42	596 110.019	–0.002	27.1385	b	581.66
46	15	32	46	14	33	596 114.773	–0.012	21.7798	b	448.52
54	15	40	54	14	41	596 129.186	–0.029	26.5412	b	565.71
47	15	33	47	14	34	596 130.619	0.015	22.3745	b	462.16
71	3	69	70	3	68	596 623.510	0.027	70.6692	a	714.15
71	2	69	70	2	68	596 626.020	0.034	70.6692	a	714.15
19	11	9	18	10	8	597 900.664	–0.033	11.3193	b	118.47
19	11	8	18	10	9	597 900.664	–0.033	11.3193	b	118.47
72	2	71	71	2	70	598 553.381	0.000	71.7923	a	720.76
72	1	71	71	1	70	598 553.381	–0.062	71.7923	a	720.76
69	6	64	68	6	63	598 564.534	0.000	68.3857	a	707.40
69	17	53	68	17	52	598 934.793	0.005	64.8151	a	878.96
69	16	54	68	16	53	598 945.751	0.012	65.2936	a	856.34
69	18	52	68	18	51	598 964.568	0.016	64.3077	a	902.93
69	15	55	68	15	54	599 006.376	0.006	65.7431	a	835.10
69	19	51	68	19	50	599 028.510	0.028	63.7712	a	928.26
69	20	50	68	20	49	599 121.682	0.000	63.2059	a	954.94
69	14	56	68	14	55	599 129.303	0.018	66.1636	a	815.25
69	21	49	68	21	48	599 240.430	0.012	62.6115	a	982.95
69	13	57	68	13	56	599 332.834	0.017	66.5553	a	796.79
69	13	56	68	13	55	599 332.834	0.009	66.5553	a	796.79
69	22	48	68	22	47	599 381.774	–0.019	61.9882	a	1012.29
69	23	47	68	23	46	599 543.527	0.006	61.3359	a	1042.96
69	12	58	68	12	57	599 644.852	0.106	66.9180	a	779.75
69	12	57	68	12	56	599 644.852	–0.067	66.9180	a	779.75
69	24	46	68	24	45	599 723.800	0.023	60.6546	a	1074.94
72	9	64	71	9	63	627 937.473	0.017	70.8821	a	798.55
71	7	64	70	7	63	628 465.846	–0.017	70.3880	a	759.72
72	8	65	71	8	64	628 562.157	–0.008	71.1101	a	787.59
32	9	24	31	8	23	628 618.468	–0.123	12.1168	b	188.10
72	9	63	71	9	62	628 623.719	0.026	70.8840	a	798.65
75	3	73	74	3	72	629 019.411	0.101	74.6680	a	795.38
76	1	75	75	1	74	630 964.181	0.130	75.7922	a	802.25
73	6	68	72	6	67	631 400.183	0.024	72.3839	a	788.91
72	8	64	71	8	63	632 450.280	0.036	71.1328	a	788.28
77	1	77	76	1	76	632 940.678	–0.025	76.9284	a	808.15
77	0	77	76	0	76	632 940.678	–0.026	76.9284	a	808.15
73	17	57	72	17	56	633 323.734	–0.010	69.0451	a	960.59
73	18	56	72	18	55	633 336.726	–0.017	68.5655	a	984.57
73	16	58	72	16	57	633 357.572	0.009	69.4975	a	937.98
73	19	55	72	19	54	633 388.758	–0.015	68.0584	a	1009.91

Table 6. continued.

Transition						Obs. Freq.	obs.- calc.	S	Dipole	E_l
J'	K'_a	K'_c	J''	K''_a	K''_c	(MHz)	(MHz)			(cm^{-1})
73	15	59	72	15	58	633 448.915	0.006	69.9224	a	916.75
73	20	54	72	20	53	633 474.038	0.003	67.5239	a	1036.59
74	5	70	73	5	69	633 495.614	0.106	73.4641	a	799.25
73	21	53	72	21	52	633 588.123	0.003	66.9621	a	1064.62
73	14	60	72	14	59	633 612.950	0.000	70.3201	a	896.91
73	22	52	72	22	51	633 727.579	–0.037	66.3729	a	1093.98
74	4	70	73	4	69	633 795.128	0.095	73.4661	a	799.19
73	13	61	72	13	60	633 871.969	0.017	70.6904	a	878.48
73	13	60	72	13	59	633 871.969	–0.016	70.6904	a	878.48
73	23	51	72	23	50	633 889.780	–0.058	65.7563	a	1124.67
73	5	68	72	5	67	633 914.899	–0.015	72.4113	a	788.32
73	24	50	72	24	49	634 072.632	–0.012	65.1123	a	1156.68
73	26	48	72	26	47	634 493.450	0.059	63.7422	a	1224.61
73	27	47	72	27	46	634 728.724	–0.010	63.0160	a	1260.52
73	11	63	72	11	62	634 830.430	0.004	71.3491	a	845.96
73	11	62	72	11	61	634 838.965	–0.003	71.3492	a	845.96
73	29	44	72	29	43	635 244.378	–0.006	61.4815	a	1336.19
18	16	3	18	15	4	635 371.283	0.049	2.7935	b	204.18
19	16	4	19	15	5	635 412.186	–0.007	3.6389	b	209.70
20	16	5	20	15	6	635 454.716	–0.018	4.4522	b	215.51
21	16	6	21	15	7	635 498.801	0.032	5.2379	b	221.62
22	16	7	22	15	8	635 544.199	–0.007	6.0000	b	228.01
23	16	8	23	15	9	635 590.985	0.034	6.7415	b	234.69
24	16	9	24	15	10	635 638.921	0.018	7.4650	b	241.66
73	10	64	72	10	63	635 650.542	0.007	71.6376	a	831.95
73	7	67	72	7	66	635 706.496	–0.009	72.2835	a	798.68
26	16	11	26	15	12	635 738.023	0.010	8.8671	b	256.48
73	10	63	72	10	62	635 748.615	0.004	71.6379	a	831.96
27	16	12	27	15	13	635 788.986	0.036	9.5491	b	264.32
14	13	1	13	12	2	635 809.046	0.010	12.5178	b	125.46
14	13	2	13	12	1	635 809.046	0.010	12.5178	b	125.46
28	16	13	28	15	14	635 840.643	–0.014	10.2205	b	272.45
30	16	15	30	15	16	635 945.873	–0.023	11.5358	b	289.59
31	16	16	31	15	17	635 999.275	0.096	12.1817	b	298.59
32	16	17	32	15	18	636 052.717	–0.012	12.8210	b	307.88
33	16	18	33	15	19	636 106.396	–0.017	13.4543	b	317.47
34	16	19	34	15	20	636 160.069	–0.024	14.0824	b	327.34
35	16	20	35	15	21	636 213.617	–0.009	14.7058	b	337.50
36	16	21	36	15	22	636 266.872	0.005	15.3249	b	347.96
37	16	22	37	15	23	636 319.646	–0.020	15.9404	b	358.70
38	16	23	38	15	24	636 371.892	0.022	16.5525	b	369.73
39	16	24	39	15	25	636 423.292	–0.031	17.1617	b	381.05
40	16	24	40	15	25	636 473.831	–0.034	17.7683	b	392.66
41	16	26	41	15	27	636 523.316	–0.016	18.3727	b	404.56
42	16	27	42	15	28	636 571.541	–0.016	18.9751	b	416.75
43	16	28	43	15	29	636 618.360	–0.011	19.5757	b	429.23
44	16	29	44	15	30	636 663.588	–0.011	20.1750	b	442.00
73	9	65	72	9	64	636 669.624	–0.012	71.8977	a	819.50
69	16	54	69	15	55	636 702.405	–0.002	35.1353	b	855.08
46	16	31	46	15	32	636 748.571	–0.014	21.3699	b	468.41
67	16	52	67	15	53	636 816.649	–0.005	33.9200	b	815.41
48	16	33	48	15	34	636 825.044	–0.015	22.5614	b	495.97
49	16	34	49	15	35	636 859.623	–0.010	23.1563	b	510.19
50	16	35	50	15	36	636 891.488	–0.020	23.7509	b	524.69
51	16	36	51	15	37	636 920.465	–0.022	24.3453	b	539.48
64	16	49	64	15	50	636 937.983	–0.001	32.1071	b	758.05
52	16	36	52	15	37	636 946.380	0.011	24.9396	b	554.57
63	16	48	63	15	49	636 966.088	–0.003	31.5052	b	739.51
53	16	38	53	15	39	636 968.944	–0.007	25.5340	b	569.94
55	16	40	55	15	41	637 003.358	–0.024	26.7235	b	601.54
61	16	46	61	15	47	637 005.301	0.033	30.3048	b	703.29
56	16	41	56	15	42	637 014.784	–0.024	27.3188	b	617.78
60	16	44	60	15	45	637 016.846	0.030	29.7060	b	685.61
57	16	42	57	15	43	637 022.055	–0.031	27.9146	b	634.31
58	16	43	58	15	44	637 024.991	–0.005	28.5110	b	651.12
73	8	66	72	8	65	637 204.547	0.015	72.1208	a	808.56

Table 6. continued.

Transition						Obs. Freq.	obs.- calc.	S	Dipole	E_l
J'	K'_a	K'_c	J''	K''_a	K''_c	(MHz)	(MHz)			(cm^{-1})
72	7	65	71	7	64	637 464.900	–0.021	71.4026	a	780.68
73	9	64	72	9	63	637 502.418	0.016	71.9001	a	819.61
19	12	7	18	11	8	638 734.557	–0.045	12.1303	b	132.90
19	12	8	18	11	7	638 734.557	–0.045	12.1303	b	132.90
78	1	78	77	1	77	641 037.722	0.030	77.9284	a	829.26
78	0	78	77	0	77	641 037.722	0.030	77.9284	a	829.26
24	11	14	23	10	13	641 477.119	–0.106	12.1537	b	148.96
75	5	71	74	5	70	641 578.592	0.114	74.4627	a	820.38
73	8	65	72	8	64	641 645.995	–0.017	72.1495	a	809.38
74	5	69	73	5	68	641 760.792	–0.005	73.4054	a	809.46
75	4	71	74	4	70	641 827.842	0.112	74.4644	a	820.33
74	17	58	73	17	57	641 912.245	–0.011	70.0988	a	981.71
74	18	57	73	18	56	641 920.591	–0.029	69.6256	a	1005.69
74	16	59	73	16	58	641 952.308	–0.027	70.5450	a	959.11
74	19	56	73	19	55	641 969.272	–0.035	69.1253	a	1031.03
74	21	54	73	21	53	642 164.880	–0.048	68.0439	a	1085.76
74	14	60	73	14	59	642 227.254	–0.007	71.3566	a	918.05
74	14	61	73	14	60	642 227.254	–0.005	71.3566	a	918.05
74	22	53	73	22	52	642 303.680	–0.042	67.4626	a	1115.12
74	23	52	73	23	51	642 465.814	–0.050	66.8543	a	1145.82
74	13	62	73	13	61	642 501.346	0.010	71.7219	a	899.63
74	13	61	73	13	60	642 501.346	–0.035	71.7219	a	899.63
39	4	36	39	3	37	182 964.487	–0.034	19.1997	b	231.84
43	4	40	43	3	41	201 516.181	–0.040	19.7405	b	279.35
70	2	68	69	3	67	588 505.206	0.000	52.2606	b	694.52
70	3	68	69	2	67	588 532.562	–0.018	52.2607	b	694.52
71	2	69	70	3	68	596 613.897	0.024	53.2654	b	714.15
71	3	69	70	2	68	596 635.621	0.025	53.2655	b	714.15

Table 7. Sample table of the predicted transitions of the ground vibrational state of $CH_3CH_2C^{15}N$.

Transition J' (K'_a, K'_c) – J'' (K''_a, K''_c)	Calc. Frequency (MHz)	Calc. Error (MHz)	S	Dipole	E_l (cm^{-1})
3 (1, 3)–2 (1, 2)	25 395.710	0.05	2.6666	A	1.62
4 (1, 3)–4 (0, 4)	25 554.136	0.05	4.3003	B	2.90
3 (0, 3)–2 (0, 2)	26 055.720	0.05	2.9994	A	0.87
3 (2, 2)–2 (2, 1)	26 083.623	0.05	1.6667	A	3.96
3 (2, 1)–2 (2, 0)	26 110.418	0.05	1.6667	A	3.96
3 (1, 2)–2 (1, 1)	26 761.502	0.05	2.6666	A	1.67
5 (1, 4)–5 (0, 5)	26 796.205	0.05	5.1207	B	4.34
6 (1, 5)–6 (0, 6)	28 339.734	0.05	5.8615	B	6.07
7 (1, 6)–7 (0, 7)	30 211.700	0.05	6.5105	B	8.09
6 (0, 6)–5 (1, 5)	31 961.207	0.05	2.8413	B	5.01
8 (1, 7)–8 (0, 8)	32 441.288	0.05	7.0582	B	10.39
4 (1, 4)–3 (1, 3)	33 853.023	0.05	3.7498	A	2.47
4 (0, 4)–3 (0, 3)	34 709.447	0.05	3.9986	A	1.74
4 (2, 3)–3 (2, 2)	34 772.635	0.05	2.9999	A	4.83
....					
59 (11, 48)–58 (10, 49)	995 315.711	0.06	18.4437	B	573.93
54 (9, 45)–54 (6, 48)	995 592.250	0.07	0.1157	B	460.59
55 (6, 50)–54 (3, 51)	995 665.199	0.07	1.2626	B	442.83
65 (10, 56)–64 (9, 55)	996 353.051	0.07	18.2257	B	666.68
65 (10, 55)–64 (9, 56)	996 527.533	0.07	18.2248	B	666.67
43 (14, 30)–42 (13, 29)	996 593.606	0.06	17.9466	B	392.48
43 (14, 29)–42 (13, 30)	996 593.606	0.06	17.9466	B	392.48
55 (5, 51)–54 (2, 52)	997 274.064	0.14	1.0781	B	434.25
38 (15, 24)–37 (14, 23)	998 380.799	0.07	17.7294	B	355.17
38 (15, 23)–37 (14, 24)	998 380.799	0.07	17.7294	B	355.17
73 (9, 65)–72 (8, 64)	999 104.052	0.08	17.3127	B	813.83
33 (16, 17)–32 (15, 18)	999 783.283	0.09	17.5672	B	326.61
33 (16, 18)–32 (15, 17)	999 783.283	0.09	17.5672	B	326.61
54 (12, 43)–53 (11, 42)	999 793.914	0.06	18.4736	B	508.77
54 (12, 42)–53 (11, 43)	999 793.924	0.06	18.4736	B	508.77

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Table 8. Sample table of the predicted transitions of the ground vibrational state of CH_3CHDCN.

Transition J' (K'_a, K'_c) – J'' (K''_a, K''_c)	Calc. Frequency (MHz)	Calc. Error (MHz)	S	Dipole	E_l (cm^{-1})
3 (1, 3)–2 (1, 2)	25 685.775	0.04	2.6666	A	1.53
6 (1, 5)–6 (0, 6)	25 869.041	0.04	5.6814	B	6.15
3 (0, 3)–2 (0, 2)	26 411.989	0.04	2.999	A	0.88
3 (2, 2)–2 (2, 1)	26 451.080	0.04	1.6667	A	3.56
3 (2, 1)–2 (2, 0)	26 489.353	0.04	1.6667	A	3.56
3 (1, 2)–2 (1, 1)	27 203.193	0.04	2.6666	A	1.58
7 (1, 6)–7 (0, 7)	28 031.338	0.04	6.2364	B	8.19
8 (1, 7)–8 (0, 8)	30 624.550	0.04	6.6694	B	10.52
9 (1, 8)–9 (0, 9)	33 684.164	0.04	6.9789	B	13.13
4 (1, 4)–3 (1, 3)	34 236.554	0.04	3.7497	A	2.38
4 (0, 4)–3 (0, 3)	35 171.176	0.04	3.9976	A	1.76
4 (2, 3)–3 (2, 2)	35 260.350	0.04	2.9999	A	4.44
19 (3, 16)–18 (4, 15)	35 268.186	0.04	3.0105	B	61.09
4 (3, 2)–3 (3, 1)	35287.953	0.04	1.7501	A	7.78
....					
69 (7, 62)–68 (6, 63)	995 929.078	0.08	4.7701	B	716.57
72 (10, 62)–71 (9, 63)	996 138.578	0.08	17.3708	B	808.21
52 (14, 39)–51 (13, 38)	996 412.325	0.12	19.3529	B	503.06
52 (14, 38)–51 (13, 39)	996 412.325	0.12	19.3529	B	503.06
43 (16, 27)–42 (15, 28)	996 549.110	0.28	19.2560	B	415.75
43 (16, 28)–42 (15, 27)	996 549.110	0.28	19.2560	B	415.75
43 (6, 37)–42 (3, 40)	996 760.122	0.06	0.10380	B	270.30
55 (7, 49)–54 (4, 50)	998 269.602	0.05	1.14220	B	454.23
30 (19, 12)–29 (18, 11)	998 460.111	0.84	19.4241	B	343.54
30 (19, 11)–29 (18, 12)	998 460.111	0.84	19.4241	B	343.54
57 (13, 45)–56 (12, 44)	999 597.559	0.09	19.3721	B	565.96
57 (13, 44)–56 (12, 45)	999 597.576	0.09	19.3721	B	565.96
26 (26, 1)–26 (25, 2)	999 902.893	5.38	0.99380	B	516.84
26 (26, 0)–26 (25, 1)	999 902.893	5.38	0.99380	B	516.84
27 (26, 2)–27 (25, 3)	999 988.702	5.38	1.95270	B	524.81
27 (26, 1)–27 (25, 2)	999 988.702	5.38	1.95270	B	524.81

The entire table is available in electronic form on the CDS website http://cdsweb.u-strasbg.fr/cgi-bin/qcat?J/A+A/493/565

Table 9. Sample table of the predicted transitions of the ground vibrational state of CH_2DCH_2CN in-plane.

Transition J' (K'_a, K'_c) – J'' (K''_a, K''_c)	Calc. Frequency (MHz)	Calc. Error (MHz)	S	Dipole	E_l (cm^{-1})
3 (0, 3)–2 (0, 2)	25 254.521	0.03	2.9995	A	0.84
3 (2, 2)–2 (2, 1)	25 278.632	0.03	1.6667	A	3.97
3 (2, 1)–2 (2, 0)	25 301.661	0.03	1.6667	A	3.97
4 (1, 3)–4 (0, 4)	25 630.983	0.03	4.3159	B	2.81
3 (1, 2)–2 (1, 1)	25 910.592	0.03	2.6666	A	1.65
5 (1, 4)–5 (0, 5)	26 781.045	0.03	5.1502	B	4.21
6 (1, 5)–6 (0, 6)	28 206.908	0.03	5.9108	B	5.89
7 (1, 6)–7 (0, 7)	29 932.070	0.03	6.5861	B	7.85
6 (0, 6)–5 (1, 5)	29 934.274	0.03	2.8151	B	4.89
8 (1, 7)–8 (0, 8)	31 982.230	0.03	7.1666	B	10.08
4 (1, 4)–3 (1, 3)	32 843.643	0.03	3.7498	A	2.43
4 (0, 4)–3 (0, 3)	33 645.594	0.03	3.9988	A	1.69
4 (2, 3)–3 (2, 2)	33 700.082	0.03	3	A	4.81
4 (3, 2)–3 (3, 1)	33 717.726	0.03	1.75	A	8.72
...					
52 (2, 50)–51 (1, 51)	996 822.420	0.19	0.1924	B	358.79
81 (22, 59)–81 (21, 60)	996 989.852	0.59	39.3263	B	1276.12
81 (22, 60)–81 (21, 61)	996 989.852	0.59	39.3263	B	1276.12
77 (8, 69)–76 (7, 70)	997 182.226	0.09	14.1792	B	863.19
82 (22, 61)–82 (21, 62)	997 192.282	0.6	39.908	B	1299.13
82 (22, 60)–82 (21, 61)	997 192.282	0.6	39.908	B	1299.13
83 (22, 61)–83 (21, 62)	997 394.781	0.62	40.4899	B	1322.41
83 (22, 62)–83 (21, 63)	997 394.781	0.62	40.4899	B	1322.41
84 (22, 62)–84 (21, 63)	997 597.271	0.63	41.072	B	1345.98
84 (22, 63)–84 (21, 64)	997 597.271	0.63	41.072	B	1345.98
58 (9, 49)–58 (6, 52)	997 690.309	0.07	0.1427	B	511.44
75 (7, 68)–74 (6, 69)	998 163.363	0.13	8.4514	B	810.36
33 (16, 17)–32 (15, 18)	998 409.251	0.04	17.5865	B	323.7
33 (16, 18)–32 (15, 17)	998 409.251	0.04	17.5865	B	323.7
52 (3, 50)–51 (0, 51)	999 456.472	0.19	0.1921	B	358.79
55 (12, 44)–54 (11, 43)	999 572.240	0.03	18.7605	B	512.11
55 (12, 43)–54 (11, 44)	999 572.246	0.03	18.7605	B	512.11

The entire table is available in electronic form on the CDS website http://cdsweb.u-strasbg.fr/cgi-bin/qcat?J/A+A/493/565

Table 10. Sample table of the predicted transitions of the ground vibrational state of CH_2DCH_2CN out-of-plane.

Transition J' (K'_a, K'_c) – J'' (K''_a, K''_c)	Calc. Frequency (MHz)	Calc. Error (MHz)	S	Dipole	E_l (cm^{-1})
3 (1, 3)–2 (1, 2)	25 366.325	0.03	2.6666	A	1.54
3 (0, 3)–2 (0, 2)	26 048.385	0.03	2.9992	A	0.87
3 (2, 2)–2 (2, 1)	26 081.805	0.03	1.6667	A	3.63
6 (1, 5)–6 (0, 6)	26 083.982	0.03	5.7568	B	6.07
3 (2, 1)–2 (2, 0)	26 114.266	0.03	1.6667	A	3.63
3 (1, 2)–2 (1, 1)	26 785.701	0.03	2.6666	A	1.58
7 (1, 6)–7 (0, 7)	28 074.467	0.03	6.3507	B	8.09
8 (1, 7)–8 (0, 8)	30 455.284	0.03	6.8307	B	10.38
9 (1, 8)–9 (0, 9)	33 259.094	0.03	7.193	B	12.96
4 (1, 4)–3 (1, 3)	33 812.231	0.03	3.7497	A	2.38
6 (0, 6)–5 (1, 5)	34 522.189	0.03	2.8968	B	4.92
4 (0, 4)–3 (0, 3)	34 693.075	0.03	3.998	A	1.74
4 (2, 3)–3 (2, 2)	34 769.082	0.03	2.9999	A	4.5
4 (3, 2)–3 (3, 1)	34 792.957	0.03	1.75	A	7.95
...					
72 (25, 47)–72 (24, 48)	998 737.270	0.4	33.1422	B	1156.68
73 (25, 49)–73 (24, 50)	998 938.927	0.41	33.7368	B	1177.83
73 (25, 48)–73 (24, 49)	998 938.927	0.41	33.7368	B	1177.83
66 (11, 56)–65 (10, 55)	998 943.870	0.03	18.9621	B	691.67
66 (11, 55)–65 (10, 56)	999 001.043	0.03	18.9619	B	691.67
74 (25, 49)–74 (24, 50)	999 141.512	0.42	34.3308	B	1199.26
74 (25, 50)–74 (24, 51)	999 141.512	0.42	34.3308	B	1199.26
75 (25, 50)–75 (24, 51)	999 344.959	0.43	34.9243	B	1220.99
75 (25, 51)–75 (24, 52)	999 344.959	0.43	34.9243	B	1220.99
53 (7, 47)–52 (4, 48)	999 517.559	0.04	0.6938	B	416.68
76 (25, 52)–76 (24, 53)	999 549.202	0.44	35.5172	B	1242.99
76 (25, 51)–76 (24, 52)	999 549.202	0.44	35.5172	B	1242.99
77 (25, 53)–77 (24, 54)	999 754.176	0.45	36.1097	B	1265.29
77 (25, 52)–77 (24, 53)	999 754.176	0.45	36.1097	B	1265.29
78 (25, 53)–78 (24, 54)	999 959.814	0.46	36.7019	B	1287.87
78 (25, 54)–78 (24, 55)	999 959.814	0.46	36.7019	B	1287.87

The entire table is available in electronic form on the CDS website http://cdsweb.u-strasbg.fr/cgi-bin/qcat?J/A+A/493/565

Table 11. Observed transitions of $CH_3CH_2C^{15}N$ (without high blend) in the frequency range of the Orion KL survey. Column 1 indicates the transition, Col. 2 provides the assumed rest frequency, Col. 3 the line strength, Col. 4 the energy of the upper level, Col. 5 the observed (centroid) frequencies assuming that the radial velocities relative to LSR are 5 km s^{-1}, Col. 6 the observed peak line temperature of main beam, and Col. 7 indicates the main beam temperature derived from the model.

Transitions J_{K_a,K_c}	Pred. Freq. (MHz)	S_{ij}	E_u/k (K)	Obs. Freq. (MHz)	Obs. T_{mb} (K)	Model T_{mb} (K)
$10_{6,5}-9_{6,4}$	87 007.366	6.40	63.0	87 007.2	0.044	0.011
$10_{6,4}-9_{6,3}$	87 007.366	6.40	63.0	[1]		
$10_{7,4}-9_{7,3}$	87 010.616	5.10	77.4	87 010.3	0.024	0.015
$10_{7,3}-9_{7,2}$	87 010.616	5.10	77.4	[1]		
$10_{5,6}-9_{5,5}$	87 011.913	7.50	50.8	[1]		
$10_{5,5}-9_{5,4}$	87 011.919	7.50	50.8	[1]		
$10_{8,2}-9_{8,1}$	87 018.779	3.60	94.1	87 019.2	0.026	0.005
$10_{8,3}-9_{8,2}$	87 018.779	3.60	94.1	[1]		
$10_{3,7}-9_{3,6}$	87 114.933	9.10	33.0	87 114.2	0.070[2]	0.009
$10_{2,8}-9_{2,7}$	87 815.417	9.60	27.5	87 814.4	0.015	0.010
$10_{1,9}-9_{1,8}$	88 914.019	9.89	24.6	88 914.3	0.015	0.011
$11_{1,11}-10_{1,10}$	92 801.263	10.9	27.9	92 803.2[2]	0.020	0.013
$11_{0,11}-10_{0,10}$	94 252.099	11.0	27.3	94 251.3	0.040[3]	0.014
$11_{2,10}-10_{2,9}$	95 397.849	10.6	32.0	95 398.2	0.010	0.013
$11_{4,7}-10_{4,6}$	95 750.117	9.55	45.4	95 750.2	0.009	0.015
$11_{3,8}-10_{3,7}$	95 868.920	10.2	37.6	95 868.2	0.015	0.012
$11_{2,9}-10_{2,8}$	96 765.809	10.6	32.2	96 764.2	0.024	0.014
$12_{0,12}-11_{0,11}$	102 578.600	12.0	32.2	102 577.1	0.042	0.018
$12_{4,9}-11_{4,8}$	104 469.699	10.7	50.4	104 470.1	0.059	0.017
$12_{4,8}-11_{4,7}$	104 472.697	10.7	50.4	[1]		
$12_{3,10}-11_{3,9}$	104 517.172	11.2	42.6	104 517.2	0.027	0.017
$12_{2,10}-11_{2,9}$	105 746.402	11.7	37.3	105 748.1	0.036	0.019
$12_{1,11}-11_{1,10}$	106 509.810	11.9	34.4	106 511.1	0.041[2]	0.020
$13_{0,13}-12_{0,12}$	110 865.655	13.0	37.6	110 867.0	0.032[2]	0.024
$13_{2,12}-12_{2,11}$	112 621.740	12.7	42.4	112 621.0	0.027	0.024
$13_{6,8}-12_{6,7}$	113 127.839	10.2	78.0	113 128.0	0.130	0.034
$13_{6,7}-12_{6,6}$	113 127.839	10.2	78.0	[1]		
$13_{8,6}-12_{8,5}$	113 129.990	8.08	109.1	[1]		
$13_{8,5}-12_{8,4}$	113 129.990	8.08	109.1	[1]		
$13_{4,9}-12_{4,8}$	113 200.301	11.8	55.8	113 201.0	0.107	0.021
$13_{3,11}-12_{3,10}$	113 245.049	12.3	48.0	113 243.9	0.095[2]	0.023
$15_{7,9}-14_{7,8}$	130 537.903	11.7	104.6	130 539.7	0.149[2]	0.054
$15_{7,8}-14_{7,7}$	130 537.903	11.7	104.6	[1]		
$15_{8,8}-14_{8,7}$	130 539.798	10.7	121.3	[1]		
$15_{8,7}-14_{8,6}$	130 539.798	10.7	121.3	[1]		
$15_{6,10}-14_{6,9}$	130 549.183	12.6	90.2	130 549.8	0.052	0.070
$15_{6,9}-14_{6,8}$	130 549.187	12.6	90.2	[1]		
$15_{9,6}-14_{9,5}$	130 550.372	9.60	140.1	[1]		
$15_{9,7}-14_{9,4}$	130 550.372	9.60	140.1	[1]		
$15_{10,6}-14_{10,5}$	130 567.307	8.33	161.2	130 567.7	0.049	0.022
$15_{10,5}-14_{10,4}$	130 567.307	8.33	161.2	[1]		
$15_{12,3}-14_{12,2}$	130 615.586	5.40	209.9	130 614.7	0.042	0.010
$15_{12,4}-14_{12,3}$	130 615.586	5.40	209.9	[1]		
$15_{4,11}-14_{4,10}$	130 673.185	13.9	67.9	130 672.7	0.073	0.034
$15_{1,14}-14_{1,13}$	132 670.810	14.9	52.3	132 670.7	0.130[4]	0.042
$15_{2,13}-14_{2,12}$	132 800.381	14.7	55.1	132 799.7	0.075	0.041
$16_{8,9}-15_{8,8}$	139 245.508	12.0	127.9	139 247.0	0.280[2]	0.098
$16_{8,8}-15_{8,7}$	139 245.508	12.0	127.9	[1]		
$16_{7,10}-15_{7,9}$	139 246.220	12.9	111.3	[1]		
$16_{7,9}-15_{7,8}$	139 246.220	12.9	111.3	[1]		
$16_{6,11}-15_{6,10}$	139 262.522	13.8	96.8	139 263.3	0.086	0.067
$16_{6,10}-15_{6,9}$	139 262.529	13.8	96.8	[1]		
$16_{10,7}-15_{10,6}$	139 271.671	9.75	167.9	139 270.8	0.078	0.029
$16_{10,6}-15_{10,5}$	139 271.671	9.75	167.9	[1]		
$16_{5,12}-15_{5,11}$	139 306.059	14.4	84.6	139 305.8	0.293[2]	0.073
$16_{5,11}-15_{5,10}$	139 306.594	14.4	84.6	[1]		
$16_{12,4}-15_{12,3}$	139 321.451	7.00	216.6	139 321.9	0.045	0.015
$16_{12,5}-15_{12,4}$	139 321.451	7.00	216.6	[1]		
$16_{1,15}-15_{1,14}$	141 313.454	15.9	59.1	141314.5	0.060	0.051
$17_{0,17}-16_{0,16}$	143 750.890	16.9	62.8	143750.6	0.18[5]1	0.056

Table 11. continued.

Transitions J_{K_a,K_c}	Pred. Freq. (MHz)	S_{ij}	E_u/k (K)	Obs. Freq. (MHz)	Obs. T_{mb} (K)	Model T_{mb} (K)
$17_{8,10}-16_{8,9}$	147 951.800	13.2	135.0	147955.6	0.256	0.064
$17_{8,9}-16_{8,8}$	147 951.800	13.2	135.0	[1]		
$17_{7,11}-16_{7,10}$	147 955.646	14.1	118.4	[1]		0.074
$17_{7,10}-16_{7,9}$	147 955.646	14.1	118.4	[1]		
$17_{9,9}-16_{9,8}$	147 959.709	12.2	153.9	[1]		0.050
$17_{9,8}-16_{9,7}$	147 959.709	12.2	153.9	[1]		
$17_{10,7}-16_{10,6}$	147 976.004	11.1	175.0	147 975.5	0.170	0.093
$17_{10,8}-16_{10,7}$	147 976.004	11.1	175.0	[1]		
$17_{6,12}-16_{6,11}$	147 977.798	14.9	103.9	147 977.5	0.192[2]	
$17_{6,11}-16_{6,10}$	147 977.813	14.9	103.9	[1]		
$17_{5,13}-16_{5,12}$	148 032.124	15.5	91.7	148 030.7	0.245	0.083
$17_{5,12}-16_{5,11}$	148 033.058	15.5	91.7	[1]		
$17_{4,14}-16_{4,13}$	148 139.616	16.1	81.7	148 137.0	0.104[2]	0.053
$17_{3,15}-16_{3,14}$	148 147.371	16.5	74.0	148 146.9	0.155[2]	0.055
$17_{4,13}-16_{4,12}$	148 174.997	16.1	81.7	148 174.4	0.158[6]	0.051
$17_{3,14}-16_{3,13}$	148 810.665	16.5	74.1	148 810.5	0.080	0.055
$17_{1,16}-16_{1,15}$	149 910.805	16.9	66.3	149 909.5	0.177[2]	0.061
$17_{2,15}-16_{2,14}$	150 846.477	16.8	69.1	150 847.5	0.135	0.060
$18_{1,18}-17_{1,17}$	151 161.544	17.9	70.3	151 170.6	0.185[7]	0.064
$18_{9,10}-17_{9,9}$	156 664.727	13.5	161.4	156 663.4	0.298[2]	0.116
$18_{9,9}-17_{9,8}$	156 664.727	13.5	161.4	[1]		
$18_{7,12}-17_{7,11}$	156 666.249	15.3	125.9	[1]		
$18_{7,11}-17_{7,10}$	156 666.250	15.3	125.9	[1]		
$18_{10,9}-17_{10,8}$	156 680.304	12.4	182.5	156 679.4	0.077	0.047
$18_{10,8}-17_{10,7}$	156 680.304	12.4	182.5	[1]		
$18_{6,13}-17_{6,12}$	156 695.130	16.0	111.5	156 693.4	0.196[2]	0.097
$18_{6,12}-17_{6,11}$	156 695.157	16.0	111.5	[1]		
$18_{4,14}-17_{4,13}$	156 939.258	17.1	89.3	156 938.4	0.133	0.060
$18_{3,15}-17_{3,14}$	157 730.365	17.5	81.6	157 729.4	0.060	0.065
$18_{2,16}-17_{2,15}$	159 848.455	17.8	76.8	159 847.4	0.105	0.071
$19_{2,18}-18_{2,17}$	163 915.948	18.8	83.4	163 916.3	0.160[8]	0.077
$19_{1,18}-18_{1,17}$	166 956.959	18.9	81.9	166 957.3	0.125	0.082
$20_{2,19}-19_{2,18}$	172 402.881	19.8	91.7	172 401.6	0.228	0.088
$20_{8,13}-19_{8,12}$	174 074.508	16.8	158.8	174 072.8	0.426[9]	0.166
$20_{8,12}-19_{8,11}$	174 074.508	16.8	158.8	[1]		
$20_{9,12}-19_{9,11}$	174 075.518	16.0	177.7	[1]		
$20_{9,11}-19_{9,10}$	174 075.518	16.0	177.7	[1]		
$20_{7,14}-19_{7,13}$	174 091.254	17.6	142.2	174 090.3	0.345[10]	0.128
$20_{7,13}-19_{7,12}$	174 091.255	17.6	142.2	[1]		
$23_{7,17}-22_{7,16}$	200 239.252	20.9	169.8	200 241.0	0.143	0.162
$23_{7,16}-22_{7,15}$	200 239.261	20.9	169.8	[1]		
$23_{12,12}-22_{12,11}$	200 251.101	16.7	275.1	200 250.9	0.136	0.064
$23_{12,11}-22_{12,10}$	200 251.101	16.7	275.1	[1]		
$23_{1,22}-22_{1,21}$	200 425.284	22.9	117.9	200 423.4[2]	0.152	0.125
$23_{16,7}-22_{16,6}$	200 442.132	11.9	398.7	200 441.0	0.016	0.020
$23_{16,8}-22_{16,7}$	200 442.132	11.9	398.7	[1]		
$23_{4,20}-22_{4,19}$	200 668.972	22.3	133.2	200 670.9	0.173[10]	0.110
$23_{2,21}-22_{2,20}$	204 419.525	22.8	121.6	204 422.9[2]	0.132	0.128
$25_{0,25}-24_{0,24}$	209 271.572	24.9	132.1	209 272.1	0.367[10]	0.138
$24_{2,22}-23_{2,21}$	213 217.376	23.8	131.8	213 215.8	0.320[11]	0.139
$25_{2,24}-24_{2,23}$	214 557.679	24.8	139.1	214 558.3	0.165	0.140
$26_{1,26}-25_{1,25}$	217 285.943	25.9	142.6	217 285.7	0.253	0.147
$26_{0,26}-25_{0,25}$	217 474.027	25.9	142.6	217 473.3	0.207	0.147
$25_{9,17}-24_{9,16}$	217 607.414	21.8	225.8	217 609.5	0.323	0.228
$25_{9,16}-24_{9,15}$	217 607.414	21.8	225.8	[1]		
$25_{10,16}-24_{10,15}$	217 609.115	21.0	246.8	[1]		
$25_{10,15}-24_{10,14}$	217 609.115	21.0	246.8	[1]		
$25_{11,15}-24_{11,14}$	217 626.225	20.2	270.1	217 626.9	0.320	0.255
$25_{11,14}-24_{11,13}$	217 626.225	20.2	270.1	[1]		
$25_{8,18}-24_{8,17}$	217 627.120	22.4	206.9	[1]		
$25_{8,17}-24_{8,16}$	217 627.120	22.4	206.9	[1]		
$25_{7,19}-24_{7,18}$	217 679.026	23.0	190.2	217 679.4	0.217	0.191
$25_{7,18}-24_{7,17}$	217 679.051	23.0	190.2	[1]		

Table 11. continued.

Transitions J_{K_a,K_c}	Pred. Freq. (MHz)	S_{ij}	E_u/k (K)	Obs. Freq. (MHz)	Obs. T_{mb} (K)	Model T_{mb} (K)
$25_{5,21}$–$24_{5,20}$	217 976.444	24.0	163.7	217 975.7	0.086	0.119
$25_{3,22}$–$24_{3,21}$	221 023.822	24.6	146.8	221 024.4	0.162	0.142
$26_{1,25}$–$25_{1,24}$	225 064.582	25.9	149.2	225 063.1	0.218	0.152
$26_{6,21}$–$25_{6,20}$	226 521.943	24.6	186.7	226 524.4[12]	0.244	0.203
$26_{6,20}$–$25_{6,19}$	226 523.621	24.6	186.7	[1]		
$26_{5,22}$–$25_{5,21}$	226 737.488	25.0	174.5	226 736.8	0.235[13]	0.127
$26_{4,22}$–$25_{4,21}$	227 585.336	25.4	164.8	227 585.5	0.498	0.139
$28_{1,28}$–$27_{1,27}$	233 761.349	27.9	164.7	233 762.4	0.239	0.163
$28_{0,28}$–$27_{0,27}$	233 886.100	27.9	164.6	233 885.3	0.151	0.164
$27_{3,25}$–$26_{3,24}$	234 807.835	26.7	168.0	234 807.4	0.325	0.154
$27_{10,18}$–$26_{10,17}$	235 016.780	23.3	269.0	235 015.4	0.150	0.146
$27_{10,17}$–$26_{10,16}$	235 016.780	23.3	269.0	[1]		
$27_{4,24}$–$26_{4,23}$	235 703.198	26.4	175.9	235 703.2	0.156	0.146
$28_{3,26}$–$27_{3,25}$	243 387.108	27.7	179.7	243 385.6	0.207	0.161
$28_{10,19}$–$27_{10,18}$	243 720.490	24.4	280.7	243 720.2	0.217	0.152
$28_{10,18}$–$27_{10,17}$	243 720.490	24.4	280.7	[1]		
$28_{9,20}$–$27_{9,19}$	243 730.327	25.1	259.6	243 730.2	0.362	0.289
$28_{9,19}$–$27_{9,18}$	243 730.327	25.1	259.6	[1]		
$28_{11,18}$–$27_{11,17}$	243 731.014	23.7	303.9	[1]		
$28_{11,17}$–$27_{11,16}$	243731.014	23.7	303.9	[1]		
$28_{12,17}$–$27_{12,16}$	243756.893	22.9	329.4	243756.3	0.200	0.102
$28_{12,16}$–$27_{12,15}$	243756.893	22.9	329.4	[1]		
$28_{6,23}$–$27_{6,22}$	244 007.283	26.7	209.7	244 007.2	0.427	0.149
$28_{6,22}$–$27_{6,21}$	244 011.067	26.7	209.7	244 010.2	0.432	0.148
$29_{6,24}$–$28_{6,23}$	252 754.799	27.8	221.8	252 755.2	0.456	0.139
$29_{6,23}$–$28_{6,22}$	252 760.349	27.8	221.8	252 760.1	0.402	0.137
$29_{5,25}$–$28_{5,24}$	253 042.421	28.1	209.7	253 041.7	0.252	0.147
$29_{4,25}$–$28_{4,24}$	254 464.800	28.4	200.1	254 464.2	0.291	0.160
$31_{1,31}$–$30_{1,30}$	258 449.466	30.9	200.7	258 449.2	0.204	0.180
$30_{6,24}$–$29_{6,23}$	261 513.668	28.8	234.4	261 512.9	0.278	0.140
$30_{2,28}$–$29_{2,27}$	264 929.014	29.8	202.0	264 929.9	0.156	0.182
$32_{0,32}$–$31_{0,31}$	266 726.277	31.9	213.5	266 725.0	0.369	0.183
$31_{3,29}$–$30_{3,28}$	269 002.338	30.7	217.2	269 002.9	0.660	0.175
$31_{8,24}$–$30_{8,23}$	269 919.627	28.9	278.3	269 918.9	0.191	0.224
$31_{8,23}$–$30_{8,22}$	269 919.638	28.9	278.3	[1]		
$31_{5,27}$–$30_{5,26}$	270 593.584	30.2	235.3	270 592.9	0.262	0.155
$31_{4,28}$–$30_{4,27}$	270 656.392	30.5	225.4	270 655.9	0.390	0.167
$31_{5,26}$–$30_{5,25}$	270 792.922	30.2	235.3	270 791.9	0.357	0.155
$33_{0,33}$–$32_{0,32}$	274 937.410	32.9	226.7	274 936.8	0.277[14]	0.185
$32_{11,22}$–$31_{11,21}$	278 531.537	28.2	354.9	278 530.1	0.736	0.247
$32_{11,21}$–$31_{11,20}$	278 531.537	28.2	354.9	[1]		
$32_{10,23}$–$31_{10,22}$	278 534.350	28.9	331.6	[1]		
$32_{10,22}$–$31_{10,21}$	278 534.350	28.9	331.6	[1]		
$32_{4,29}$–$31_{4,28}$	279 370.232	31.5	238.8	279 270.2	0.556	0.301
$32_{5,28}$–$31_{5,27}$	279 371.886	31.2	248.7	[1]		
$32_{5,27}$–$31_{5,26}$	279 633.253	31.2	248.7	279 632.8	0.384	0.157