

The Millimeter- and Submillimeter-Wave Spectrum of *trans*-Ethyl Alcohol

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The rotational-torsional spectrum of the *trans* rotational isomer of ethyl alcohol was investigated in the 65–350 GHz frequency region. A total of 481 ground state transitions over a range of J and K_a values up to 33 and 10, respectively, were measured and assigned. Doublets or triplets arising from the A and E torsional states of the $v=0$ torsional level of the three-fold-symmetric methyl internal rotation have been resolved in 168 of these transitions. Internal rotation theory predicts a significant number of c -type E -state transitions normally forbidden, but allowed when the rotational asymmetry operators mix E -state rotational-torsional levels. Over 40 of these transitions have been observed. The newly measured transitions, along with the results of many previous measurements, have been analyzed using an IAM internal rotation Hamiltonian and a Watson A -reduced Hamiltonian to determine the rotational, centrifugal distortion, and torsional constants. The IAM analysis accounts for all of the analyzed transitions in the *trans* isomer, but for some applications the asymmetric rotor analysis is a satisfactory description of the molecule. The J and K_a limits where the *trans* isomer can be analyzed without considering interactions with the *gauche* states are also discussed. Predicted frequencies for transitions unaffected by the *gauche* states are presented through 600 GHz using the constants determined by this work. ©1995 American Institute of Physics and American Chemical Society.

Key words: ethanol; intensities; interstellar molecules; microwave spectra; molecular constants; radio astronomy; rotational spectrum; internal rotation.

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1. Introduction

The microwave spectrum of ethyl alcohol has been the subject of previous investigations by several groups. Early work on the *trans* rotational isomer, or rotamer, was carried out by researchers in Belgium, the USSR, and Japan [1–3]. These different research groups were originally interested primarily in determining the structure of the molecule [1–21]. The first extensive set of microwave measurements included 96 transitions and was the result of a series of investigations by Michielsen-Effinger [17]. A total of 38 of these assigned transitions were confirmed with a double resonance technique by Seipt [22]. A study of the *trans* isomer in the first excited hydroxyl torsional state, the first excited methyl torsional state, and the $\nu=1$ state of the CCO bend was conducted by Sasada [23–24]. The existence of *gauche* rotamers of the hydroxyl torsional motion, corresponding to secondary minima in the torsional potential, was discussed in several early papers, and a few transitions belonging to these rotamers were assigned [3, 4, 7, 9]. The first major attempt at assigning rotational-torsional spectra involving the *gauche* rotamers was made by Kakar and Seipt using double resonance techniques [25]. In a thorough study, Kakar and Quade [26] determined the potential barriers to OH torsional and methyl motions, as well as the *gauche* dipole moment components [26]. In a previous Journal of Physical and Chemical Reference Data review article, Lovas [27] collected and analyzed with a Watson Hamiltonian most of the previously reported *trans* spectral lines including many previously unpublished transitions. Also reported in this work were the first *trans* transitions with resolved methyl torsional splittings, along with information on the *gauche* states and other isotopes [27]. Predicted transition frequencies for selected transitions through $J = 25$ and 300 GHz based on data below 130 GHz were given for the *trans* rotamer. In this article, we extend the measured frequency range for this rotamer to 350 GHz and the range of predicted transition frequencies through 600 GHz.

Ethyl alcohol in its *trans* rotational isomer has been observed in several warm, dense interstellar molecular clouds, following the initial observation by Zuckerman *et al.* in Sgr B2 [28,29]. It is believed to be responsible for a number of observed but heretofore unassigned transitions in the submillimeter-wave region [30]. Therefore, a systematic study of the rotational spectrum in the millimeter-wave and submillimeter-wave regions is necessary to confirm the hypothesis. There are several competing theories regarding the interstellar formation of ethanol and other large organo-oxygen molecules [31]. In particular, it is believed that these molecules can be formed both in the gas phase and on grain mantles. For the latter mechanism, warming temperatures associated with star formation are needed to drive the material into the gas phase where it can be detected via rotational transitions. The dual formation mechanisms suggest that detection should be possible in both warm and cold interstellar regions. All of the confirmed astronomical observations to date are of the *trans* isomer; however, it should be possible to detect the transitions in the *gauche* isomers as well since they lie only about 60 Kelvin above the *trans* isomer. A complete

study of the *gauche* rotamers will thus be important for astronomical observations and assignments of this molecule, and a useful probe of temperature in star forming regions.

2. Theory

A near prolate asymmetric top, the ethyl alcohol molecule possesses in addition two large amplitude internal motions: the threefold symmetric internal rotation of the methyl group and the asymmetric internal rotation of the hydroxyl group. The motion of the methyl group is hindered by a high barrier ($V_3 \approx 1164 \text{ cm}^{-1}$) to threefold internal rotation [20,27], which can be analyzed with either a principal axis method (PAM) or an internal axis method (IAM) for describing the internal rotation. The threefold symmetry leads to torsional substates of *A* and *E* symmetry in the C_3 group. Rotational transitions within these substates occur at nearly identical frequencies due to the high barrier, although small *A-E* splittings can often be resolved. In addition, transitions normally forbidden in asymmetric tops occur in the *E* torsional substates. The asymmetric internal rotation of the hydroxyl group possesses an intermediate-size barrier with three potential minima, as can be seen in Fig. 1. The global minimum is referred to as the *trans* configuration or rotamer, whereas the secondary minima are referred to as *gauche* configurations or rotamers. Figure 2 shows the positions of the hydroxyl group for the three potential minima, looking down the CO bond. The potential leads to a pattern of three torsional substates; the higher the potential barriers, the greater the degree of localization of the wave functions centered on the potential minima. For the ground level, the lowest torsional substate is the *trans* state with two *gauche* states, the *gauche+* and *gauche-*, at higher energies. The absolute values of the wave functions for the *gauche* states contain peaks at both *gauche* positions, with the + and - designations referring to symmetric and antisymmetric linear combinations. Kakar and Quade determined that the *gauche+* and *gauche-* states are split by 3.2 cm^{-1} and lie $41.2 \pm 5.0 \text{ cm}^{-1}$ above the *trans* state [26]. Figure 3 shows how rotational levels in the ground vibrational state are split by hydroxyl and methyl torsional motions. The 41.2 cm^{-1} energy difference between *trans* and *gauche* states is large enough to leave a significant number of *trans* rotational levels unaffected by the *gauche* rotational levels, but the larger rotational constants for the *trans* rotamer lead to the fact that at high enough rotational energy the *trans* and *gauche* rotational levels will start to overlap. As a result, rotational transitions in the *trans* state should be unperturbed for a fairly wide range of *J* and K_a values. However, at high *J* and K_a values, the *trans* rotamer rotational energy levels will eventually cross the *gauche* rotamer levels with comparable quantum numbers resulting in the Coriolis-like perturbations that are observed in the *trans* spectrum. The 3.2 cm^{-1} energy difference between the *gauche* states results in strong perturbations beginning at low *J* values, requiring the perturbations to be considered in the analysis of the *gauche* spectrum [26].

The *trans* isomer of ethyl alcohol has a dipole moment that lies almost exactly on the *b*-axis, making *a*-type transitions either very weak or undetectable. Although some *a*-type transitions might be observable ($\mu \approx 0.046 D$), we and earlier

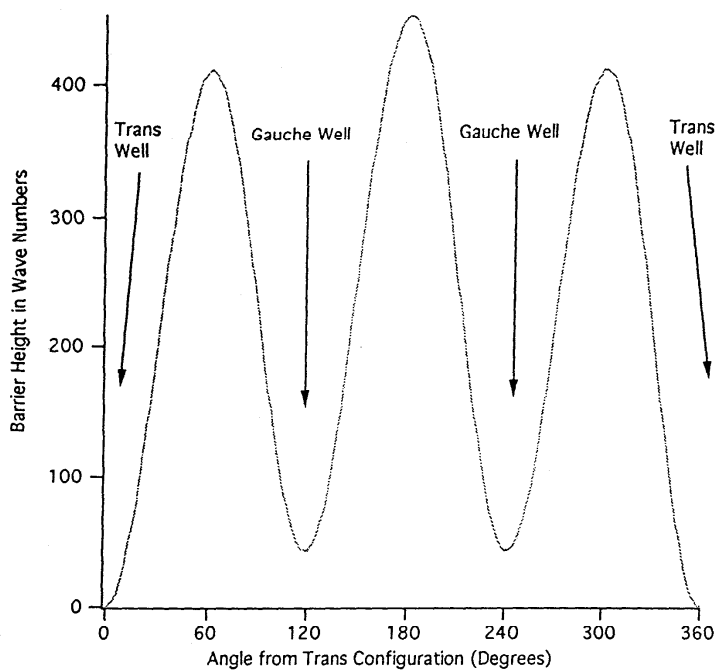


FIG. 1. Hydroxyl barrier. The potential energy for internal rotation of the hydroxyl group in ethyl alcohol is shown as a function of torsional angle. The two different *gauche* wells are of equal depth and lie above the *trans* well [26].

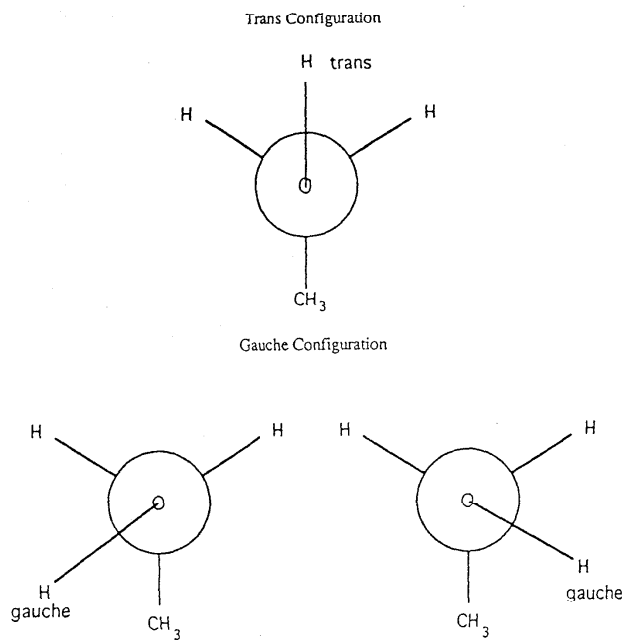


FIG. 2. Hydroxyl position. The position of the hydroxyl group looking down the CO bond in ethyl alcohol is shown for the *trans* and *gauche* configurations. The *gauche+* state is characterized by the symmetric superposition of wave functions peaking at the *gauche* hydrogen positions while the *gauche-* state is characterized by the asymmetric superposition.

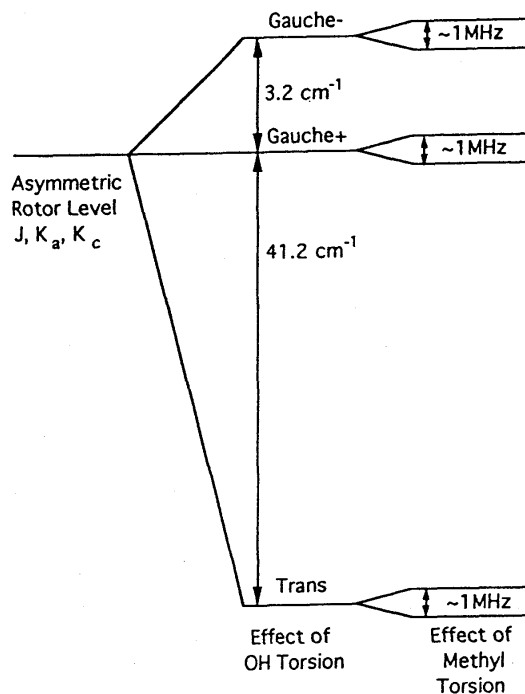


FIG. 3. Ground state rotational-torsional energy levels. The splittings of asymmetric rotor levels in the ground vibrational state of ethanol due to the effects of OH and methyl torsional motions are depicted. The splittings due to the methyl torsional motion are representative values.

groups have been unable to detect them. The c -component of the dipole moment is zero by symmetry. Most of the *trans* b -type transitions are very strong with the exception of some P/R branches which have small transition moments. The *gauche* isomers have a nearly zero dipole component in the b -direction so that no b -type transitions have been unambiguously observed. Pure rotational transitions (i.e., transitions within the *gauche+* or *gauche-* states) have a -type selection rules whereas transitions between *gauche+* and *gauche-* states are allowed by the non-zero moment in the c -direction [26]. The change in dipole moment direction in the different rotamers suggests that the dipole moment in ethyl alcohol is primarily associated with the internally rotating hydroxyl group.

The selection rules deduced from a consideration of the rigid-body rotational and hydroxyl torsional motions must be slightly modified when methyl internal rotation is included. In particular, despite the absence of a dipole moment along the c -axis, c -type transitions can be observed in the *trans* rotamer if the methyl torsional motion lies in an E torsional substate and the asymmetry splitting in either the upper or lower set of K_a doublets is comparable in size with the internal rotation splitting. This effect arises here from the competition between the asymmetry-induced splitting, leading to parity doublets with wave functions $|K_a\rangle \pm | -K_a\rangle$ (neglecting the mixing of other K_a values), and torsional-rotational interaction, leading to wave functions characterized by $|K_a\rangle$ and $| -K_a\rangle$. For prolate molecules with b -type spectra, the mixing produces c -type transitions with considerable intensity. Both the intensities of c -type

transitions and the frequency splittings between b -type and c -type spectral lines require an internal rotation analysis. For ethanol, the effect is largest when the asymmetry splittings are on the order of 1 MHz, which is comparable to the methyl internal rotation effect. The mixing of parity states described here is not the only mechanism leading to c -type transitions; high order torsional-rotational interaction can actually reverse the $-K_a, +K_a$ ordering of the E -state K_a doublets and transfer intensity from b -type to c -type transitions completely if asymmetric top notation is utilized [32].

3. Experimental

The ethanol sample used was reagent grade obtained from commercial sources. The sample was introduced into sample cells which ranged from one to four meters in length. Measurements were made at pressures from 6 to 35 mTorr. The small methyl splittings were resolved at low pressures and small frequency modulation. The weaker transitions were observed at higher pressures and with larger modulation. The spectra were recorded on three different spectrometer systems. Spectra between 78 and 117 GHz were measured with the spectrometer at the Physikalisch Chemisches Institute of the Justus Liebig Universität in Giessen, Germany. This spectrometer uses a KVARZ millimeter-wave synthesizer as a source. Other spectra were recorded with either a tripled YIG oscillator amplified by a TWT amplifier and multiplied by a Gordy type harmonic generator or with a 55 GHz klystron and a similar harmonic generator. InSb hot electron bolometers

The measurement accuracy is better than 50 kHz for the strong split transitions and better than 100 kHz for all transitions measured in this work.

Extensive measurements were made between 65 and 350 GHz, including re-measurement of many previously reported transitions in an effort to resolve the methyl splittings, many of which are detectable in the Doppler limit. A total of 481 transitions, including 168 with resolved methyl torsional splittings, have been measured and analyzed. In the case of small asymmetry splitting of the K_a doublets, extra transitions were often observed and assigned to *c*-type methyl internal rotation-allowed transitions as shown in Fig. 4 and discussed above. All split transitions require the methyl internal rotation to be considered for detailed analysis. The large number of *trans* transitions which are not resolvable into *A* and *E* components can be analyzed more simply via a standard asymmetric top treatment, in which the split transitions can also be considered by suitable averaging [27].

Many transitions of the *gauche* and *trans* isomers exhibiting perturbations were measured and assigned, but they are not included in the present analysis since they require a proper treatment of the hydroxyl torsional motion, and its kinetic and potential interaction with other motions. Indeed, in addition to an extension of the *trans* rotational spectrum to higher frequency, another purpose of this work was to determine the

range of J and K_a values in which the *trans* state could be analyzed without considering interactions with the *gauche* rotamers in the ground OH torsional state. The existence of unsplit transitions [17, 22] that cannot be analyzed accurately with a simple asymmetric top analysis has been known for some time, as has the likely origin of the problem. More data were needed to confirm the hypothesis, necessitating the measurement of a significant number of new transitions.

4. Analysis

The present analysis of the spectrum of the unperturbed rotational transitions in the *trans* state was performed in two stages. The first step was to account for the methyl splittings and the *c*-type transitions. An internal axis method (IAM) torsional analysis was used to predict all the transitions in *trans*-ethanol, whether resolved or not; however, for some purposes, such as astronomical searches, the IAM analysis is unnecessary, since the methyl torsional splittings will not be resolved. As a result, a standard asymmetric top analysis using a Watson *A*-reduced Hamiltonian [37] was performed on all the unresolved transitions and the average of the split (*A,E*) *b*-type transitions. This analysis was used to generate predictions for astronomical use.

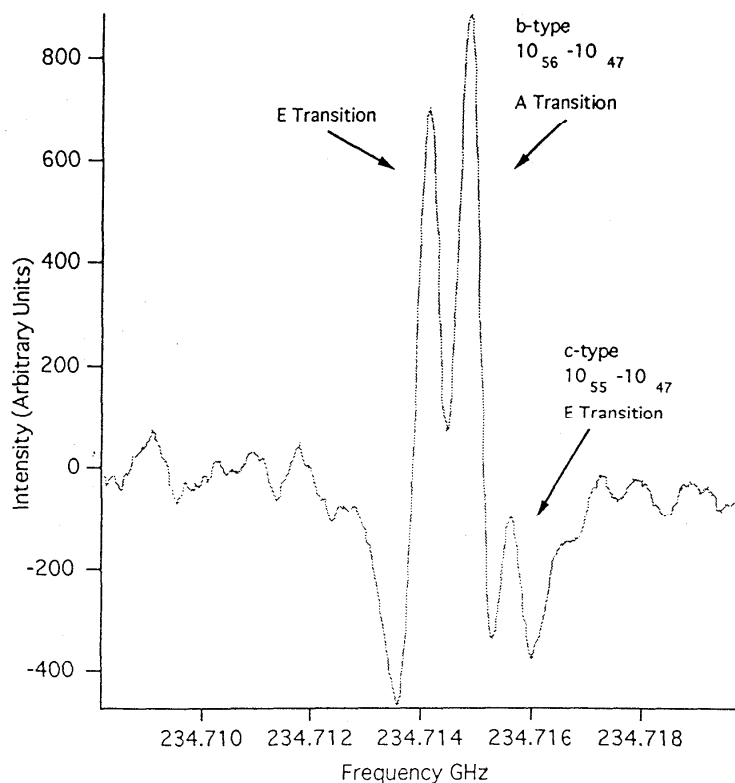


Fig. 4. Triplet spectrum. A completely resolved *Q*-branch spectral triplet at 234.7 GHz is shown. The splitting of the *b*-type transitions in the *A* and *E* torsional substates as well as the appearance of a *c*-type spectral transition is caused by the effects of methyl internal rotation.

4.1. IAM Analysis

The IAM Hamiltonian is similar to that used for methanol [38] although, for ethanol, rotational-torsional energy levels have been calculated only for the lowest torsional state and asymmetric rotor notation utilized. A similar analysis can be found in [39]. A total of 220 *A*-state and 261 *E*-state transitions with quantum numbers in the range $J \leq 30$ and $K_a \leq 7$ including the 115 transitions reported by Lovas [27] were fit to a root-mean-square (RMS) deviation of 97 kHz. The transitions used in this analysis are given in Table 1 along with the calculated frequencies and residuals. The rotational constants A, B, C, D_{ab} ; four of the five fourth-order distortion constants ($\Delta_{JK}, \Delta_J, \Delta_K, \delta_J$); three sixth-order distortion constants; the threefold potential barrier V_3 ; and the unitless internal rotation parameter ρ were determined. The parameter F , the reduced rotational constant for torsional motion, was fixed at the value calculated from the molecular structure determined by Culot [20]. The parameter D_{ab} is in principle calculable from a combination of other molecular parameters and is highly correlated with A and B . The fit is slightly better if D_{ab} is varied, but the uncertainty in A and B is much larger as a result. Due to the high barrier and the small value of ρ , it is not surprising that none of the high-order interaction constants between torsion and rotation is determinable or needed [38]. The internal rotation analysis correctly predicts the *E*-state mixings and the intensities of the *c*-type *E*-state transitions.

The constants determined from the IAM analysis are given in Table 2. The only constant that can be compared directly with constants from previous PAM analyses is V_3 , the threefold potential barrier. Our threefold barrier of 1173.7 cm^{-1} agrees within uncertainties to previous values of 1169.2 cm^{-1} and 1164.3 cm^{-1} [20, 24]. The analysis does not include any coupling between the OH and CH₃ internal motions or V_6 effects, which clearly influence the barrier height. In addition, our analysis cannot fit the effects of the perturbations with the *gauche* states, and several transitions were excluded for this reason. Predictions of transition frequencies and *A*-*E* splittings through $J=30$ are available upon request.

4.2. Asymmetric Rotor Analysis

In addition to the IAM analysis, virtually all of the measured *b*-type *trans* lines were fit with a Watson *A*-reduced Hamiltonian in the I' representation [37]. In this analysis, the *b*-type transitions with resolved methyl internal rotation splittings were averaged so as to resemble blends. The analysis contained a total of 557 transitions, including 481 from this work. The measured transitions, predicted frequencies, residuals, S values, and energy levels are given in Table 3. Intensities can be obtained by multiplying the S values by the square of the *b*-component of the dipole moment ($\mu_b = 1.44 D$). The energy of the primed (upper) state is given. Table 3 also includes a list of *trans* isomer predictions with uncertainties to 600 GHz that do not exhibit the effects of perturbations with the *gauche* states (see the discussion below). A total of 16 parameters were determined with this analysis and are shown in Table 4. This table also shows

parameters determined from an updated analysis of lower frequency data [27]. Comparison between the two sets of parameters shows some discrepancy in the sextic terms. The RMS deviation of 111 kHz is a little larger than the measurement accuracy, but the analysis does show some systematic error at low J values, where the methyl splittings tend to be measurable. The fit also has difficulty accounting for the regions where the *c*-type transitions occur because the average *b*-type frequency is not where it would be in the absence of *E* state torsional mixing. Another problem exists at high J and K_a limits, where it is possible that the *trans* rotational levels are starting to show small shifts due to interactions with the increasingly nearby *gauche* rotational levels of comparable quantum numbers. These effects probably cause some increase in RMS deviation, but appear to be random due to the differing magnitudes of the interactions. Transitions at high J and K_a values that are systematically shifted and could not be fit without considering interactions with the *gauche* states are not included in the analysis and have been excluded from the predictions in Table 3. Predictions at frequencies above 600 GHz are available from the authors but must be used cautiously.

5. Discussion

The maximum J value to which the *trans* state can be analyzed without considering the effects of the *gauche* states is given in Table 5 as a function of K_a . As K_a increases, the maximum value of J decreases. There is some K_c dependence to the onset of the perturbations within a given K_a value, so the values in Table 5 are approximate. In general, for a given K_a value, once the perturbations start several J levels can be followed in a slowly diverging pattern before large deviations occur. Presumably at still higher values of J , the perturbations will decrease in size. An analysis of the strongly perturbed *trans* rotational levels and the rotational levels in the *gauche* states will require either a three-state Coriolis perturbation Hamiltonian or an IAM Hamiltonian which contains the asymmetric hydroxyl internal rotation and its interactions—both kinetic and potential. The two analyses we have performed on rotational-torsional transitions in the *trans* isomer account satisfactorily for all the *trans* transitions observed that do not exhibit perturbations. Predictions based on the constants within the range of J and K_a values given should be accurate enough to assign many new astronomical lines through 600 GHz. Indeed, assignments of 14 new submillimeter-wave lines of ethanol in a warm molecular cloud [40] have been made very recently based on our measurements and predictions.

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TABLE 1. Transitions exhibiting resolved methyl torsional splittings in the ground vibrational state of *trans*-ethanol

TS	J'	K_a'	K_c'	J''	K_a''	K_c''	Freq. obs. (MHz)	Freq. cal. (MHz)	Obs-cal (MHz)
A	11	3	9	10	4	6	10528.950	10528.909	0.041
E	11	3	9	10	4	6	10529.350	10529.281	0.069
A	6	1	6	5	2	3	11770.850	11770.857	-0.007
E	6	1	6	5	2	3	11771.100	11771.114	-0.014
A	14	4	11	13	5	8	12016.800	12016.761	0.039
E	14	4	11	13	5	8	12017.150	12017.101	0.049
A	14	4	10	13	5	9	12726.150	12726.079	0.071
E	14	4	10	13	5	9	12726.500	12726.467	0.033
A	17	5	13	16	6	10	12843.250	12843.335	-0.085
E	17	5	13	16	6	10	12843.500	12843.580	0.080
A	17	5	12	16	6	11	13014.050	13014.019	0.031
E	17	5	12	16	6	11	13014.400	13014.365	0.035
A	11	3	8	10	4	7	13214.100	13214.032	0.068
E	11	3	8	10	4	7	13214.500	13214.419	0.081
A	20	6	15	19	7	12	13489.300	13489.366	-0.066
E	20	6	15	19	7	12	13489.500	13489.519	-0.019
A	20	6	14	19	7	13	13528.200	13528.193	0.007
E	20	6	14	19	7	13	13528.400	13528.436	-0.036
A	8	2	6	7	3	5	15518.400	15518.466	-0.066
E	8	2	6	7	3	5	15518.750	15518.796	-0.046
A	5	1	4	4	2	3	17818.500	17818.569	-0.069
E	5	1	4	4	2	3	17818.700	17818.779	-0.079
E	2	2	1	3	1	2	22367.200	22366.998	0.202
A	2	2	1	3	1	2	22367.400	22367.236	0.164
E	17	7	11	18	6	12	22520.450	22520.429	0.021
A	17	7	11	18	6	12	22520.850	22520.808	0.042
E	17	7	10	18	6	12	22520.850	22520.838	0.012
E	17	7	11	18	6	13	22531.350	22531.336	0.014
A	17	7	10	18	6	13	22531.800	22531.814	-0.014
E	17	7	10	18	6	13	22531.800	22531.745	0.055
E	14	6	9	15	5	10	23127.600	23127.696	-0.096
A	14	6	9	15	5	10	23128.100	23128.246	-0.146
E	14	6	8	15	5	10	23128.500	23128.653	-0.153
A	9	2	8	8	3	5	23130.100	23130.150	-0.050
E	9	2	8	8	3	5	23130.450	23130.480	-0.030
F	14	6	9	15	5	11	23176.700	23176.560	0.140
A	14	6	8	15	5	11	23177.600	23177.618	-0.018
E	14	6	8	15	5	11	23177.600	23177.516	0.084
A	7	1	7	6	2	4	23263.450	23263.365	0.085
E	7	1	7	6	2	4	23263.700	23263.629	0.071
E	5	3	3	6	2	4	23493.600	23493.405	0.195
A	5	3	3	6	2	4	23493.950	23493.769	0.181
E	11	5	7	12	4	8	23665.200	23665.060	0.140
A	11	5	7	12	4	8	23665.650	23665.595	0.055
E	11	5	6	12	4	9	23876.850	23876.821	0.029
A	11	5	6	12	4	9	23877.050	23877.073	-0.023
E	8	4	5	9	3	6	23947.350	23947.546	-0.196
A	8	4	5	9	3	6	23947.800	23948.002	-0.202
E	8	4	4	9	3	7	24789.250	24789.205	0.045
A	8	4	4	9	3	7	24789.650	24789.559	0.091
E	5	3	2	6	2	5	26409.400	26409.438	-0.038
A	5	3	2	6	2	5	26409.700	26409.776	-0.076
A	12	3	10	11	4	7	28075.200	28075.169	0.031
E	12	3	10	11	4	7	28075.600	28075.531	0.069
E	2	2	0	3	1	3	29700.550	29700.423	0.127
A	2	2	0	3	1	3	29700.750	29700.666	0.084
A	15	4	12	14	5	9	30044.500	30044.684	-0.184
E	15	4	12	14	5	9	30044.800	30045.020	0.220
A	18	5	14	17	6	11	30976.850	30976.873	-0.023
E	18	5	14	17	6	11	30977.100	30977.130	-0.030
A	15	4	11	14	5	10	31258.000	31257.762	0.238
E	15	4	11	14	5	10	31258.400	31258.120	0.280
A	18	5	13	17	6	12	31276.500	31276.381	0.119
E	18	5	13	17	6	12	31276.800	31276.681	0.119
A	21	6	16	20	7	13	31616.900	31617.049	-0.149

TABLE 1. Transitions exhibiting resolved methyl torsional splittings in the ground vibrational state of *trans*-ethanol — Continued

TS	J'	K_a'	K_c'	J''	K_a''	K_c''	Freq. obs. (MHz)	Freq. cal. (MHz)	Obs-cal (MHz)
E	21	6	16	20	7	13	31617.100	31617.214	-0.114
A	21	6	15	20	7	14	31686.600	31686.402	0.198
E	21	6	15	20	7	14	31686.850	31686.603	0.247
A	12	3	9	11	4	8	32483.700	32483.575	0.125
E	12	3	9	11	4	8	32484.000	32483.944	0.056
A	8	1	8	7	2	5	33260.700	33260.561	0.139
E	8	1	8	7	2	5	33261.000	33260.833	0.167
A	9	2	7	8	3	6	36143.200	36143.362	-0.162
E	9	2	7	8	3	6	36143.500	36143.677	-0.177
A	6	1	5	5	2	4	38674.600	38674.444	0.156
E	6	1	5	5	2	4	38674.800	38674.640	0.160
E	16	7	10	17	6	11	40431.900	40431.848	0.052
A	16	7	10	17	6	11	40432.300	40432.290	0.010
E	16	7	9	17	6	11	40432.300	40432.270	0.030
E	16	7	10	17	6	12	40437.300	40437.370	-0.070
A	16	7	9	17	6	12	40437.800	40437.820	-0.020
E	16	7	9	17	6	12	40437.800	40437.793	0.007
E	13	6	8	14	5	9	41048.100	41048.128	-0.028
A	13	6	8	14	5	9	41048.800	41048.807	-0.007
E	13	6	7	14	5	9	41049.000	41048.994	0.006
E	13	6	8	14	5	10	41072.750	41072.738	0.012
A	13	6	7	14	5	10	41073.600	41073.604	-0.004
E	13	6	7	14	5	10	41073.600	41073.604	-0.004
A	9	1	9	8	2	6	41580.050	41579.869	0.181
E	9	1	9	8	2	6	41580.350	41580.153	0.197
E	10	5	6	11	4	7	41620.200	41620.207	-0.007
A	10	5	6	11	4	7	41620.900	41620.922	-0.022
E	10	5	5	11	4	7	41621.650	41621.631	0.019
E	10	5	6	11	4	8	41725.700	41725.608	0.092
A	10	5	5	11	4	8	41727.100	41727.129	-0.029
E	10	5	5	11	4	8	41727.100	41727.032	0.068
E	7	4	4	8	3	5	42049.500	42049.494	0.006
A	7	4	4	8	3	5	42050.050	42050.061	-0.011
E	7	4	3	8	3	5	42052.550	42052.540	0.010
E	4	3	2	5	2	3	42075.850	42075.749	0.101
A	4	3	2	5	2	3	42076.250	42076.167	0.083
E	7	4	3	8	3	6	42472.800	42472.711	0.089
A	7	4	3	8	3	6	42473.100	42472.974	0.126
A	13	3	11	12	4	8	45459.600	45459.435	0.165
E	13	3	11	12	4	8	45460.000	45459.784	0.216
A	16	4	13	15	5	10	48102.500	48102.541	-0.041
E	16	4	13	15	5	10	48102.900	48102.865	0.035
A	19	5	15	18	6	12	49193.800	49193.946	-0.146
E	19	5	15	18	6	12	49194.100	49194.196	-0.096
A	19	5	14	18	6	13	49702.200	49702.336	-0.136
E	19	5	14	18	6	13	49702.500	49702.606	-0.106
A	13	3	10	12	4	9	52372.300	52372.311	-0.011
E	13	3	10	12	4	9	52372.700	52372.661	0.039
A	11	2	10	10	3	7	53359.200	53359.016	0.184
E	11	2	10	10	3	7	53359.500	53359.330	0.170
E	9	2	7	9	1	8	65484.491	65484.515	-0.024
A	9	2	7	9	1	8	65484.687	65484.698	-0.011
E	10	2	8	10	1	9	65937.626	65937.653	-0.027
A	10	2	8	10	1	9	65937.808	65937.828	-0.020
A	5	0	5	4	1	4	65997.071	65997.265	-0.194
E	5	0	5	4	1	4	65997.285	65997.324	-0.039
A	17	4	14	16	5	11	66159.087	66159.108	-0.021
E	17	4	14	16	5	11	66159.372	66159.414	-0.042
A	12	2	11	11	3	8	67140.222	67140.202	0.020
E	12	2	11	11	3	8	67140.523	67140.509	0.014
E	7	2	5	7	1	6	67186.459	67186.493	-0.034
A	7	2	5	7	1	6	67186.689	67186.695	-0.006
E	11	2	9	11	1	10	67484.976	67485.000	-0.024
A	11	2	9	11	1	10	67485.158	67485.169	-0.011
A	20	5	16	19	6	13	67490.707	67490.829	-0.122

TABLE 1. Transitions exhibiting resolved methyl torsional splittings in the ground vibrational state of *trans*-ethanol — Continued

TS	J'	K_a'	K_c'	J''	K_a''	K_c''	Freq. obs. (MHz)	Freq. cal. (MHz)	Obs-cal (MHz)
E	20	5	16	19	6	13	67490.960	67491.064	-0.104
A	20	5	15	19	6	14	68328.143	68328.192	-0.049
E	20	5	15	19	6	14	68328.388	68328.437	-0.049
E	6	2	4	6	1	5	68934.784	68934.793	-0.009
A	6	2	4	6	1	5	68935.014	68935.005	0.009
E	12	2	10	12	1	11	70262.008	70262.027	-0.019
A	12	2	10	12	1	11	70262.166	70262.192	-0.026
E	5	2	3	5	1	4	70976.721	70976.719	0.002
A	5	2	3	5	1	4	70976.950	70976.941	0.009
E	10	1	9	10	0	10	71971.752	71971.693	0.059
A	10	1	9	10	0	10	71971.935	71971.869	0.066
A	14	3	11	13	4	10	73001.824	73001.750	0.074
E	14	3	11	13	4	10	73002.164	73002.081	0.083
E	4	2	2	4	1	3	73081.103	73081.101	0.002
A	4	2	2	4	1	3	73081.349	73081.331	0.018
E	13	2	11	13	1	12	74380.602	74380.619	-0.017
A	13	2	11	13	1	12	74380.768	74380.781	-0.013
E	3	2	1	3	1	2	75035.929	75035.906	0.023
A	3	2	1	3	1	2	75036.160	75036.143	0.017
E	14	7	7	15	6	9	76070.628	76070.985	-0.357
E	14	7	8	15	6	10	76072.077	76071.940	0.137
E	2	2	0	2	1	1	76662.376	76662.341	0.035
A	2	2	0	2	1	1	76662.614	76662.579	0.035
A	15	3	13	14	4	10	79367.396	79367.378	0.018
E	15	3	13	14	4	10	79367.715	79367.695	0.020
A	13	2	12	12	3	9	79762.477	79762.456	0.021
E	13	2	12	12	3	9	79762.781	79762.756	0.025
A	11	2	9	10	3	8	79799.054	79799.022	0.032
E	11	2	9	10	3	8	79799.337	79799.300	0.037
E	2	2	1	2	1	2	80266.140	80266.099	0.041
A	2	2	1	2	1	2	80266.296	80266.356	-0.060
E	3	2	2	3	1	3	82115.615	82115.577	0.038
A	3	2	2	3	1	3	82115.874	82115.833	0.041
E	11	1	10	11	0	11	82650.273	82650.211	0.062
A	11	1	10	11	0	11	82650.482	82650.409	0.073
A	18	4	15	17	5	12	84170.015	84170.092	-0.077
E	18	4	15	17	5	12	84170.307	84170.378	-0.071
E	4	2	3	4	1	4	84595.738	84595.693	0.045
A	4	2	3	4	1	4	84595.998	84595.951	0.047
A	21	5	17	20	6	14	85858.104	85858.264	-0.160
E	21	5	17	20	6	14	85858.305	85858.481	-0.176
A	21	5	16	20	6	15	87199.970	87200.008	-0.038
E	21	5	16	20	6	15	87200.160	87200.230	-0.070
E	5	2	4	5	1	5	87715.968	87715.928	0.040
A	5	2	4	5	1	5	87716.236	87716.190	0.046
A	18	4	14	17	5	13	89060.666	89060.625	0.041
E	18	4	14	17	5	13	89060.964	89060.915	0.049
A	14	2	13	13	3	10	91007.580	91007.559	0.021
E	14	2	13	13	3	10	91007.879	91007.853	0.026
E	6	2	5	6	1	6	91484.968	91484.995	-0.027
A	6	2	5	6	1	6	91485.311	91485.263	0.048
E	13	7	6	14	6	8	93811.770	93812.242	-0.472
A	13	7	7	14	6	8	93812.554	93812.477	0.077
E	13	7	7	14	6	9	93812.554	93812.704	-0.150
A	13	7	6	14	6	9	93813.117	93812.997	0.120
A	12	1	11	12	0	12	94278.203	94278.364	-0.161
E	12	1	11	12	0	12	94278.203	94278.140	0.063
E	10	6	5	11	5	6	94378.069	94378.080	-0.011
A	10	6	5	11	5	6	94379.059	94379.055	0.004
E	10	6	5	11	5	7	94380.525	94380.520	0.005
A	10	6	4	11	5	7	94381.287	94381.224	0.063
A	15	3	12	14	4	11	94477.778	94477.702	0.076
E	15	3	12	14	4	11	94478.076	94478.012	0.064
E	7	5	3	8	4	4	94894.969	94894.939	0.030
A	7	5	3	8	4	4	94896.196	94896.046	0.150

TABLE I. Transitions exhibiting resolved methyl torsional splittings in the ground vibrational state of *trans*-ethanol — Continued

TS	J'	K'_a	K'_c	J''	K''_a	K''_c	Freq. obs. (MHz)	Freq. cal. (MHz)	Obs-cal (MHz)
E	7	5	3	8	4	5	94903.276	94903.252	0.024
A	7	5	2	8	4	5	94904.341	94904.275	0.066
A	4	4	1	5	3	2	95337.414	95337.084	0.330
E	4	4	0	5	3	2	95337.414	95337.331	0.083
E	4	4	1	5	3	3	95361.810	95361.757	0.053
A	4	4	0	5	3	3	95363.236	95362.881	0.355
E	4	4	0	5	3	3	95363.236	95363.141	0.095
A	16	3	14	15	4	11	95650.241	95650.259	-0.018
E	16	3	14	15	4	11	95650.548	95650.558	-0.010
E	7	2	6	7	1	7	95909.095	95909.059	0.036
A	7	2	6	7	1	7	95909.350	95909.334	0.016
A	24	2	23	23	3	20	99896.059	99896.104	-0.045
E	24	2	23	23	3	20	99896.487	99896.504	-0.017
A	15	2	14	14	3	11	100659.995	100659.982	0.013
E	15	2	14	14	3	11	100660.305	100660.272	0.033
E	8	2	7	8	1	8	100989.963	100989.922	0.041
A	8	2	7	8	1	8	100990.24	100990.204	0.037
A	19	4	16	18	5	13	102075.871	102076.036	-0.165
E	19	4	16	18	5	13	102076.116	102076.300	-0.184
E	15	3	12	15	2	13	102283.493	102283.420	0.073
A	15	3	12	15	2	13	102283.658	102283.631	0.027
A	12	2	10	11	3	9	102764.231	102764.189	0.042
E	12	2	10	11	3	9	102764.479	102764.446	0.033
E	14	3	11	14	2	12	105064.211	105064.186	0.025
A	14	3	11	14	2	12	105064.411	105064.418	-0.007
E	13	1	12	13	0	13	106649.354	106649.292	0.062
A	13	1	12	13	0	13	106649.603	106649.542	0.061
E	9	2	8	9	1	9	106723.414	106723.373	0.041
A	9	2	8	9	1	9	106723.701	106723.663	0.038
E	13	3	10	13	2	11	108438.488	108438.469	0.019
A	13	3	10	13	2	11	108438.669	108438.722	-0.053
A	16	2	15	15	3	12	108524.376	108524.366	0.010
E	16	2	15	15	3	12	108524.676	108524.654	0.022
A	19	4	15	18	5	14	109394.729	109394.702	0.027
E	19	4	15	18	5	14	109395.001	109394.968	0.033
A	17	3	15	16	4	12	11287.023	11287.096	-0.073
E	17	3	15	16	4	12	11287.303	11287.376	-0.073
E	12	3	9	12	2	10	112129.406	112129.446	-0.040
A	12	3	9	12	2	10	112129.681	112129.720	-0.039
E	6	5	2	7	4	3	112522.434	112522.394	0.040
A	6	5	2	7	4	3	112523.663	112523.627	0.036
E	6	5	1	7	4	3	112523.663	112523.671	-0.008
E	6	5	2	7	4	4	112525.463	112525.440	0.023
A	6	5	1	7	4	4	112526.378	112526.373	0.005
E	2	2	1	1	1	0	112807.060	112807.007	0.053
A	2	2	1	1	1	0	112807.287	112807.264	0.023
E	10	2	9	10	1	10	113097.924	113097.885	0.039
A	10	2	9	10	1	10	113098.231	113098.185	0.046
A	22	2	21	21	3	18	113308.806	113308.855	-0.049
E	22	2	21	21	3	18	113309.175	113309.208	-0.033
E	2	2	0	1	1	1	114064.861	114064.768	0.093
A	2	2	0	1	1	1	114065.025	114065.017	0.008
A	17	2	16	16	3	13	114443.823	114443.822	0.001
E	17	2	16	16	3	13	114444.121	114444.112	0.009
E	11	3	8	11	2	9	115865.976	115866.022	-0.046
A	11	3	8	11	2	9	115866.266	115866.315	-0.049
A	16	3	13	15	4	12	116874.959	116874.877	0.082
E	16	3	13	15	4	12	116875.225	116875.163	0.062
A	21	2	20	20	3	17	117498.084	117498.073	0.011
E	21	2	20	20	3	17	117498.084	117498.406	-0.322
E	9	3	6	9	2	7	122550.497	122550.547	-0.050
A	9	3	6	9	2	7	122550.800	122550.872	-0.072
E	8	3	5	8	2	6	125173.012	125173.045	-0.033
A	8	3	5	8	2	6	125173.374	125173.383	-0.009
A	18	3	16	17	4	13	126099.604	126099.760	-0.156

TABLE I. Transitions exhibiting resolved methyl torsional splittings in the ground vibrational state of *trans*-ethanol — Continued

TS	J'	K_a'	K_c'	J''	K_a''	K_c''	Freq. obs. (MHz)	Freq. cal. (MHz)	Obs-cal (MHz)
E	18	3	16	17	4	13	126099.876	126100.022	-0.146
E	7	3	4	7	2	5	127214.970	127215.002	-0.032
A	7	3	4	7	2	5	127215.332	127215.348	-0.016
E	12	2	11	12	1	12	127683.273	127683.247	0.026
A	12	2	11	12	1	12	127683.614	127683.570	0.044
E	6	3	3	6	2	4	128689.487	128689.495	-0.008
A	6	3	3	6	2	4	128689.844	128689.847	-0.003
E	3	2	2	2	1	1	129077.517	129077.495	0.022
A	3	2	2	2	1	1	129077.778	129077.746	0.032
E	5	3	2	5	2	3	129665.552	129665.547	0.005
A	5	3	2	5	2	3	129665.909	129665.896	0.013
A	3	3	0	3	2	1	130545.153	130545.147	0.006
E	3	3	0	3	2	1	130545.153	130545.096	0.057
E	3	3	1	3	2	2	130754.966	130754.920	0.046
A	3	3	1	3	2	2	130755.634	130755.615	0.019
E	4	3	2	4	2	3	130871.282	130871.247	0.035
A	4	3	2	4	2	3	130871.703	130871.676	0.027
E	5	3	3	5	2	4	131102.847	131102.838	0.009
A	5	3	3	5	2	4	131103.233	131103.218	0.015
E	6	3	4	6	2	5	131502.569	131502.562	0.007
A	6	3	4	6	2	5	131502.946	131502.927	0.019
E	7	3	5	7	2	6	132128.881	132128.908	-0.027
A	7	3	5	7	2	6	132129.257	132129.265	-0.008
E	15	1	14	15	0	15	132727.490	132727.472	0.018
A	15	1	14	15	0	15	132727.832	132727.780	0.052
E	3	2	1	2	1	2	132935.025	132935.006	0.019
A	3	2	1	2	1	2	132935.282	132935.264	0.018
E	8	3	6	8	2	7	133043.782	133043.806	-0.024
A	8	3	6	8	2	7	133044.054	133044.156	-0.102
E	9	3	7	9	2	8	134310.188	134310.227	-0.039
A	9	3	7	9	2	8	134310.554	134310.570	-0.016
E	13	2	12	13	1	13	135830.460	135830.428	0.032
A	13	2	12	13	1	13	135830.822	135830.764	0.058
E	10	3	8	10	2	9	135989.738	135989.787	-0.049
A	10	3	8	10	2	9	135990.094	135990.123	-0.029
E	11	3	9	11	2	10	138140.450	138140.491	-0.041
A	11	3	9	11	2	10	138140.797	138140.821	-0.024
E	17	3	14	16	4	13	140225.040	140224.984	0.056
E	17	3	14	16	4	13	140225.297	140225.243	0.054
E	12	3	10	12	2	11	140814.639	140814.699	-0.060
A	12	3	10	12	2	11	140814.980	140815.023	-0.043
E	20	2	18	20	1	19	142046.183	142046.325	-0.142
A	20	2	18	20	1	19	142046.436	142046.562	-0.126
E	13	3	11	13	2	12	144057.327	144057.382	-0.055
A	13	3	11	13	2	12	144057.668	144057.700	-0.032
E	14	2	13	14	1	14	144492.917	144492.880	0.037
A	14	2	13	14	1	14	144493.297	144493.231	0.066
E	4	2	3	3	1	2	144733.982	144733.967	0.015
A	4	2	3	3	1	2	144734.214	144734.213	0.001
E	16	1	15	16	0	16	146021.885	146021.881	0.004
A	16	1	15	16	0	16	146022.248	146022.219	0.029
E	14	3	12	14	2	13	147904.636	147904.688	-0.052
A	14	3	12	14	2	13	147904.976	147905.000	-0.024
E	15	3	13	15	2	14	152382.798	152382.835	-0.037
A	15	3	13	15	2	14	152383.125	152383.143	-0.018
E	15	2	14	15	1	15	153622.958	153622.942	0.016
A	15	2	14	15	1	15	153623.339	153623.308	0.031
E	16	3	14	16	2	15	157507.345	157507.350	-0.005
A	16	3	14	16	2	15	157507.612	157507.655	-0.043
E	17	1	16	17	0	17	159270.982	159271.001	-0.019
A	17	1	16	17	0	17	159271.386	159271.367	0.019
A	25	5	21	24	6	18	159559.479	159559.163	0.316
E	25	5	21	24	6	18	159559.693	159559.285	0.408
E	17	4	13	17	3	14	161917.119	161916.952	0.167
A	17	4	13	17	3	14	161917.286	161917.219	0.067

TABLE 1. Transitions exhibiting resolved methyl torsional splittings in the ground vibrational state of *trans*-ethanol — Continued

TS	J'	K_a'	K_c'	J''	K_a''	K_c''	Freq. obs. (MHz)	Freq. cal. (MHz)	Obs-cal (MHz)
E	16	2	15	16	1	16	163169.653	163169.638	0.015
A	16	2	15	16	1	16	163170.069	163170.020	0.049
E	17	3	15	17	2	16	163282.630	163282.657	-0.027
A	17	3	15	17	2	16	163282.950	163282.958	-0.008
E	16	4	12	16	3	13	166439.457	166439.393	0.064
A	16	4	12	16	3	13	166439.737	166439.685	0.052
E	18	3	16	18	2	17	169702.042	169702.055	-0.013
A	18	3	16	18	2	17	169702.345	169702.355	-0.010
E	22	2	20	22	1	21	170035.784	170036.049	-0.265
A	22	2	20	22	1	21	170036.040	170036.324	-0.284
E	15	4	11	15	3	12	170381.446	170381.447	-0.001
A	15	4	11	15	3	12	170381.766	170381.762	0.004
E	18	1	17	18	0	18	172372.000	172372.033	-0.033
A	18	1	17	18	0	18	172372.440	172372.428	0.012
E	17	2	16	17	1	17	173080.689	173080.666	0.023
A	17	2	16	17	1	17	173081.117	173081.065	0.052
E	5	2	3	4	1	4	173391.250	173391.191	0.059
A	5	2	3	4	1	4	173391.416	173391.461	-0.045
E	8	4	4	8	3	5	182229.851	182229.912	-0.061
A	8	4	4	8	3	5	182230.238	182230.278	-0.040
E	11	4	8	11	3	9	182409.869	182409.947	-0.078
A	11	4	8	11	3	9	182410.279	182410.334	-0.055
E	10	4	7	10	3	8	182450.810	182450.903	-0.093
A	10	4	7	10	3	8	182451.250	182451.306	-0.056
E	12	4	9	12	3	10	182453.970	182454.047	-0.077
A	12	4	9	12	3	10	182454.374	182454.418	-0.044
E	9	4	6	9	3	7	182538.000	182538.073	-0.073
A	9	4	6	9	3	7	182538.451	182538.497	-0.046
E	13	4	10	13	3	11	182630.564	182630.619	-0.055
A	13	4	10	13	3	11	182630.941	182630.975	-0.034
E	8	4	5	8	3	6	182641.703	182641.771	-0.068
A	8	4	5	8	3	6	182642.198	182642.237	-0.039
E	7	4	4	7	3	5	182741.307	182741.335	-0.028
A	7	4	4	7	3	5	182741.881	182741.909	-0.028
E	7	4	3	7	3	5	182744.327	182744.381	-0.054
E	6	4	3	6	3	3	182747.238	182747.221	0.017
E	6	4	3	6	3	4	182824.376	182824.377	-0.001
A	6	4	3	6	3	4	182825.158	182825.201	-0.043
E	6	4	2	6	3	4	182825.921	182825.919	0.002
E	5	4	2	5	3	2	182859.945	182859.965	-0.020
A	5	4	1	5	3	2	182861.206	182861.181	0.025
E	5	4	2	5	3	3	182885.782	182885.775	0.007
A	5	4	2	5	3	3	182886.782	182886.812	-0.030
E	4	4	1	4	3	1	182919.162	182919.170	-0.008
A	4	4	0	4	3	1	182920.438	182920.375	0.063
E	4	4	0	4	3	1	182920.438	182920.554	-0.116
E	4	4	1	4	3	2	182925.760	182925.746	0.014
A	4	4	1	4	3	2	182926.911	182926.813	0.098
E	14	4	11	14	3	12	182994.392	182994.407	-0.015
A	14	4	11	14	3	12	182994.743	182994.748	-0.005
E	3	3	1	2	2	0	183170.099	183170.074	0.025
A	3	3	1	2	2	0	183170.772	183170.782	-0.010
E	3	3	0	2	2	0	183171.980	183171.643	0.337
E	3	3	1	2	2	1	183212.416	183212.435	-0.019
E	18	2	17	18	1	18	183304.348	183304.309	0.039
A	18	2	17	18	1	18	183304.743	183304.726	0.017
E	21	1	20	21	0	21	210390.923	210390.916	0.007
A	21	1	20	21	0	21	210391.301	210391.385	-0.084
E	21	2	20	21	1	21	215375.428	215375.356	0.072
A	21	2	20	21	1	21	215375.855	215375.830	0.025
E	22	1	21	22	0	22	222643.952	222643.960	-0.008
A	22	1	21	22	0	22	222644.380	222644.451	-0.071
E	12	5	8	12	4	9	234255.000	234255.014	-0.014
A	12	5	8	12	4	9	234255.321	234255.452	-0.131
E	11	5	7	11	4	8	234509.291	234509.359	-0.068

TABLE 1. Transitions exhibiting resolved methyl torsional splittings in the ground vibrational state of *trans*-ethanol — Continued

TS	J'	K_a'	K_c'	J''	K_a''	K_c''	Freq. obs. (MHz)	Freq. cal. (MHz)	Obs-cal (MHz)
A	11	5	7	11	4	8	234509.838	234509.892	-0.054
E	11	5	6	11	4	8	234511.780	234511.800	-0.020
E	10	5	6	10	4	6	234664.764	234664.836	-0.072
A	10	5	5	10	4	6	234666.273	234666.371	-0.098
E	10	5	5	10	4	6	234666.273	234666.261	0.012
E	10	5	6	10	4	7	234714.202	234714.304	-0.102
A	10	5	6	10	4	7	234714.939	234715.011	-0.072
E	10	5	5	10	4	7	234715.735	234715.728	0.007
E	23	1	22	23	0	23	234725.345	234725.388	-0.043
A	23	1	22	23	0	23	234725.858	234725.900	-0.042
E	9	5	5	9	4	5	234851.838	234851.897	-0.059
A	9	5	4	9	4	5	234853.026	234853.087	-0.061
E	9	5	4	9	4	5	234853.026	234853.129	-0.103
E	9	5	5	9	4	6	234873.131	234873.217	-0.086
A	9	5	5	9	4	6	234874.091	234874.098	-0.007
E	8	5	4	8	4	4	234983.240	234983.139	0.101
A	8	5	3	8	4	4	234984.238	234984.274	-0.036
E	8	5	3	8	4	4	234984.238	234984.371	-0.133
E	8	5	4	8	4	5	234991.406	234991.452	-0.046
A	8	5	4	8	4	5	234992.404	234992.407	-0.003
E	7	5	3	7	4	3	235072.279	235072.311	-0.032
A	7	5	2	7	4	3	235073.491	235073.537	-0.046
E	7	5	2	7	4	3	235073.491	235073.567	-0.076
E	7	5	3	7	4	4	235075.285	235075.357	-0.072
A	7	5	3	7	4	4	235076.248	235076.263	-0.015
E	6	5	2	6	4	2	235130.624	235130.113	0.511
A	6	5	1	6	4	2	235131.505	235131.595	-0.090
E	6	5	2	6	4	3	235131.505	235131.655	-0.150
E	6	5	1	6	4	2	235131.505	235131.390	0.115
A	6	5	2	6	4	3	235132.356	235132.342	0.014
E	5	5	1	5	4	2	235166.636	235166.653	-0.017
E	5	5	0	5	4	1	235166.636	235166.574	0.062
E	24	1	23	24	0	24	246663.333	246663.451	-0.118
A	24	1	23	24	0	24	246663.897	246663.983	-0.086
A	4	4	1	3	3	0	252951.382	252951.412	-0.030
E	4	4	1	3	3	1	252951.382	252951.526	-0.144
E	4	4	0	3	3	0	252951.382	252951.341	0.041
A	4	4	0	3	3	1	252952.404	252952.352	0.052
E	25	1	24	25	0	25	258484.364	258484.396	-0.032
A	25	1	24	25	0	25	258484.950	258484.947	0.003
E	25	2	24	25	1	25	260007.434	260007.401	0.033
A	25	2	24	25	1	25	260008.022	260007.950	0.072
E	26	1	25	26	0	26	270211.012	270211.034	-0.022
A	26	1	25	26	0	26	270211.642	270211.604	0.038
E	5	4	2	4	3	1	270443.174	270443.187	-0.013
A	5	4	2	4	3	1	270444.339	270444.305	0.034
E	5	4	1	4	3	1	270444.339	270444.563	-0.224
E	5	4	2	4	3	2	270449.768	270449.763	0.005
A	5	4	1	4	3	2	270450.945	270450.910	0.035
E	5	4	1	4	3	2	270450.945	270451.139	-0.194
E	26	2	25	26	1	26	271324.143	271324.115	0.028
A	26	2	25	26	1	26	271324.766	271324.681	0.085
E	27	1	26	27	0	27	281862.314	281862.340	-0.026
A	27	1	26	27	0	27	281862.958	281862.927	0.031
E	27	2	26	27	1	27	282671.554	282671.496	0.058
A	27	2	26	27	1	27	282672.149	282672.080	0.069
E	15	6	10	15	5	10	286117.079	286116.855	0.224
A	15	6	9	15	5	10	286118.554	286118.477	0.077
E	15	6	9	15	5	10	286118.554	286118.282	0.272
A	15	6	10	15	5	11	286166.139	286166.126	0.013
E	15	6	9	15	5	11	286167.416	286167.145	0.271
A	14	6	8	14	5	9	286437.960	286437.894	0.066
E	14	6	8	14	5	9	286437.960	286437.787	0.173
E	13	6	8	13	5	8	286691.119	286691.176	-0.057
A	13	6	7	13	5	8	286692.129	286692.066	0.063

TABLE 1. Transitions exhibiting resolved methyl torsional splittings in the ground vibrational state of *trans*-ethanol — Continued

TS	J'	K_a'	K_c'	J''	K_a''	K_c''	Freq. obs. (MHz)	Freq. cal. (MHz)	Obs-cal (MHz)
E	13	6	7	13	5	8	286692.129	286692.042	0.087
E	13	6	8	13	5	9	286702.901	286702.935	-0.034
A	13	6	8	13	5	9	286703.713	286703.570	0.143
E	13	6	7	13	5	9	286703.713	286703.801	-0.088
E	12	6	7	12	5	7	286890.950	286891.051	-0.101
A	12	6	6	12	5	7	286891.976	286891.927	0.049
E	12	6	6	12	5	7	286891.976	286891.929	0.047
E	12	6	7	12	5	8	286896.323	286896.393	-0.070
A	12	6	7	12	5	8	286897.188	286897.078	0.110
E	12	6	6	12	5	8	286897.188	286897.271	-0.083
E	11	6	6	11	5	6	287045.574	287045.674	-0.100
A	11	6	5	11	5	6	287046.644	287046.633	0.011
E	11	6	5	11	5	6	287046.644	287046.580	0.064
E	11	6	6	11	5	7	287048.059	287048.115	-0.056
A	11	6	6	11	5	7	287048.861	287048.768	0.093
E	11	6	5	11	5	7	287048.861	287049.020	-0.159
E	6	4	3	5	3	2	287917.406	287917.501	-0.095
A	6	4	3	5	3	2	287918.309	287918.352	-0.043
E	6	4	2	5	3	2	287919.212	287919.043	0.169
E	6	4	3	5	3	3	287943.287	287943.312	-0.025
A	6	4	2	5	3	3	287944.832	287944.882	-0.050
E	6	4	2	5	3	3	287944.832	287944.853	-0.021
E	30	1	29	30	0	30	316501.850	316501.898	-0.048
A	30	1	29	30	0	30	316502.515	316502.535	-0.020
E	30	2	29	30	1	30	316804.487	316804.498	-0.011
A	30	2	29	30	1	30	316805.158	316805.133	0.025

Notes: line frequencies below 60 GHz are from Ref. [27]. The symbol "TS" refers to the symmetry of the methyl torsional substate. The measurement accuracy is better than 50 kHz for the strong split transitions and better than 100 kHz for all transitions measured in this work.

TABLE 2. Internal rotation constants for the ground vibrational state of *trans*-ethanol

Contant	Value (MHz unless stated)	Uncertainty (1 σ)	Units
A	34106.87786	(96000)	
B	10137.36448	(96000)	
C	8133.409785	(1200)	
D_{ab}	4409.960070	(2600000)	
F	6.47394	(Fixed)	cm ⁻¹
ρ	0.18687	(210)	unitless
V_s	1173.76	(220)	cm ⁻¹
Δ_{JK}	-0.06455670	(4600)	
Δ_j	0.009453058	(2700)	
Δ_K	0.30251487	(11000)	
δ_j	0.002198832	(820)	
$H_{JK} \times 10^6$	-0.46099	(3400)	
$H_{KJ} \times 10^6$	-16.73719	(61000)	
$H_K \times 10^6$	20.19872	(180000)	

Notes: The number of significant figures for each constant is necessary to reproduce calculated frequencies to 10 kHz. The uncertainties are written without decimal points and refer to the right-most significant figures of the respective constants.

TABLE 3. Observed and calculated transition frequencies for the ground vibrational state of *trans*-¹²CH₃¹²CH₂¹⁶OH

Transition		Freq. obs. (MHz)	Freq. cal. (MHz)	Uncertainty (MHz)	Int. (S)	Energy 'state (cm ⁻¹)	Ref.
J' K _a ' K _c '	J'' K _a '' K _c ''						
4(2 2) - 5(1 5)			1015.371	0.011	0.488	9.341	
3(2 2) - 4(1 3)			2540.060	0.011	0.423	6.988	
21(2 19) - 22(1 22)			2634.307	0.037	0.109	141.385	
26(5 22) - 27(2 25)			4081.020	0.048	0.315	227.579	
6(3 4) - 7(2 5)			4333.800	0.013	0.725	20.113	
18(7 12) - 19(6 13)			4537.139	0.016	2.057	142.615	
18(7 11) - 19(6 14)			4558.191	0.016	2.057	142.615	
15(6 10) - 16(5 11)			5113.203	0.011	1.722	101.492	
15(6 9) - 16(5 12)			5206.947	0.011	1.722	101.492	
9(4 6) - 10(3 7)			5558.667	0.012	1.054	40.239	
12(5 8) - 13(4 9)			5563.615	0.010	1.388	67.366	
12(5 7) - 13(4 10)			5960.738	0.010	1.387	67.366	
8(2 7) - 7(3 4)			7035.609	0.012	0.903	24.446	
9(4 5) - 10(3 8)			7109.780	0.012	1.050	40.240	
21(1 21) - 20(2 18)			7459.851	0.034	0.119	129.175	
25(4 22) - 26(1 25)			7502.179	0.044	0.248	204.465	
26(4 23) - 27(1 26)			7865.891	0.051	0.246	219.696	
24(4 21) - 25(1 24)			8234.732	0.038	0.248	189.809	
27(4 24) - 28(1 27)			9224.334	0.060	0.242	235.499	
2(0 2) - 1(1 1)		9388.250	9388.284	-0.034	0.535	1.748	27
6(3 3) - 7(2 6)			9516.959	0.013	0.704	20.116	
23(4 20) - 24(1 23)			10164.569	0.034	0.244	175.393	
11(3 9) - 10(4 6)		10529.220	10529.140	0.080	1.260	46.441	27
28(4 25) - 29(1 28)			11476.608	0.070	0.237	251.872	
6(1 6) - 5(2 3)		11771.020	11770.983	0.037	0.603	12.675	27
14(4 11) - 13(5 8)		12017.300	12016.962	0.338	1.600	75.372	27
14(4 10) - 13(5 9)		12726.380	12726.298	0.082	1.602	75.395	27
17(5 13) - 16(6 10)		12843.450	12843.428	0.022	1.936	111.280	27
22(2 20) - 23(1 23)			12884.166	0.041	0.100	154.391	
17(5 12) - 16(6 11)		13014.250	13014.131	0.119	1.937	111.286	
11(3 8) - 10(4 7)		13214.250	13214.267	-0.017	1.269	46.529	27
22(4 19) - 23(1 22)			13390.901	0.031	0.237	162.234	
20(6 15) - 19(7 12)		13489.370	13489.399	-0.029	2.271	154.179	27
20(6 14) - 19(7 13)		13528.270	13528.238	0.032	2.271	154.180	27
3(2 1) - 4(1 4)		14897.850	14897.765	0.085	0.333	6.995	27
25(5 21) - 26(2 24)			15444.789	0.042	0.278	212.288	
8(2 6) - 7(3 5)		15518.630	15518.642	-0.012	0.950	24.723	27
20(1 20) - 19(2 17)			17175.672	0.032	0.133	117.595	
5(1 4) - 4(2 3)		17818.630	17818.667	-0.037	0.705	9.915	27
21(4 18) - 22(1 21)			18009.465	0.029	0.225	149.320	
20(8 12) - 21(7 15)		21899.500	21899.415	0.085	2.177	178.451	17
2(2 1) - 3(1 2)		22367.270	22367.130	0.140	0.182	5.329	27
17(7 11) - 18(6 12)		22520.670	22520.810	-0.140	1.843	132.088	27
17(7 10) - 18(6 13)		22531.690	22531.819	-0.129	1.843	132.088	27
31(4 28) - 32(1 31)			22620.821	0.122	0.217	304.373	
31(2 30) - 30(3 27)			23070.753	0.116	0.242	285.710	
23(2 21) - 24(1 24)			23094.349	0.045	0.093	167.937	
14(6 9) - 15(5 10)		23127.900	23128.118	-0.218	1.509	92.719	27
9(2 8) - 8(3 5)		23130.330	23130.347	-0.017	1.089	29.670	27
14(6 8) - 15(5 11)		23177.420	23177.495	-0.075	1.509	92.717	27
7(1 7) - 6(2 4)		23263.620	23263.499	0.121	0.671	16.599	27
5(3 3) - 6(2 4)		23493.720	23493.590	0.130	0.509	16.607	27
11(5 7) - 12(4 8)		23665.430	23665.364	0.066	1.175	60.348	27
11(5 6) - 12(4 9)		23876.850	23876.846	0.004	1.175	60.348	27
8(4 5) - 9(3 6)		23947.640	23947.765	-0.125	0.841	34.977	27
8(4 4) - 9(3 7)			24789.321	0.012	0.839	34.977	
19(1 19) - 18(2 16)			26278.274	0.032	0.150	106.557	
5(3 2) - 6(2 5)		26409.500	26409.590	0.090	0.501	16.607	27
1(1 0) - 1(0 1)		26756.350	26756.320	0.030	1.500	1.476	27
3(0 3) - 2(1 2)		27919.650	27919.752	-0.102	1.117	3.493	27
2(1 1) - 2(0 2)		28014.100	28014.146	-0.046	2.441	2.683	27
12(3 10) - 11(4 7)		28075.470	28075.391	0.079	1.468	53.466	27
24(5 20) - 25(2 23)			28697.189	0.038	0.237	197.588	
2(2 0) - 3(1 3)		29700.620	29700.552	-0.068	0.158	5.240	27

TABLE 3. Observed and calculated transition frequencies for the ground vibrational state of *trans*-¹²CH₃¹³CH₂¹⁶OH — Continued

Transition		Freq. obs.	Freq. cal.	Uncertainty	Int.	Energy	Ref.
<i>J'</i>	<i>K_a' K_c'</i>	(MHz)	(MHz)	(MHz)	(<i>S</i>)	'statc (cm ⁻¹)	
3(1 2) - 3(0 3)		29979.400	29979.354	0.046	3.295	4.493	27
15(4 12) - 14(5 9)		30044.700	30044.861	-0.161	1.813	84.167	27
18(5 14) - 17(6 11)		30977.020	30976.940	0.080	2.150	121.833	27
15(4 11) - 14(5 10)		31258.270	31257.972	0.298	1.816	84.207	27
18(5 13) - 17(6 12)		31276.700	31276.481	0.219	2.151	121.843	27
21(6 16) - 20(7 13)		31616.970	31617.098	-0.128	2.485	166.485	27
21(6 15) - 20(7 14)		31686.690	31686.472	0.218	2.485	166.488	27
19(4 16) - 20(1 19)			31772.929	0.027	0.188	125.248	
12(3 9) - 11(4 8)		32483.900	32483.807	0.093	1.485	53.609	27
4(1 3) - 4(0 4)		32742.800	32742.797	0.003	4.027	6.904	27
24(2 22) - 25(1 25)			33109.611	0.050	0.088	182.019	
8(1 8) - 7(2 5)		33260.900	33260.703	0.197	0.690	21.078	27
18(1 18) - 17(2 15)			34534.254	0.032	0.172	96.062	
30(2 29) - 29(3 26)			34958.466	0.096	0.259	268.336	
9(2 7) - 8(3 6)		36143.400	36143.535	-0.135	1.184	30.090	27
5(1 4) - 5(0 5)		36417.100	36417.202	-0.102	4.611	9.915	27
17(3 15) - 18(0 18)			38567.076	0.027	0.102	97.330	
10(2 9) - 9(3 6)		38626.300	38626.495	-0.195	1.254	35.466	27
6(1 5) - 5(2 4)		38674.730	38674.537	0.193	1.026	13.523	27
18(3 16) - 19(0 19)			38769.450	0.028	0.101	107.837	
16(3 14) - 17(0 17)			39397.543	0.027	0.101	87.397	
19(8 12) - 20(7 13)		39801.700	39802.066	-0.366	1.965	166.758	17
19(8 11) - 20(7 14)		39803.300	39803.261	0.039	1.965	166.758	17
19(3 17) - 20(0 20)			39918.547	0.029	0.099	118.917	
16(7 10) - 17(6 11)		40432.150	40432.314	-0.164	1.632	122.149	27
16(7 9) - 17(6 12)		40437.650	40437.846	-0.196	1.632	122.149	27
13(6 8) - 14(5 9)		41048.550	41048.674	-0.124	1.298	84.534	27
18(4 15) - 19(1 18)			41062.710	0.027	0.164	114.094	
13(6 7) - 14(5 10)		41073.390	41073.473	-0.083	1.298	84.534	27
6(1 5) - 6(0 6)		41124.950	41125.084	-0.134	5.029	13.523	27
15(3 13) - 16(0 16)			41344.124	0.026	0.098	78.043	
9(1 9) - 8(2 6)		41580.250	41580.021	0.229	0.667	26.110	27
10(5 6) - 11(4 7)		41620.620	41620.687	0.067	0.965	53.918	27
17(1 17) - 16(2 14)			41722.016	0.032	0.200	86.110	
10(5 5) - 11(4 8)		41726.900	41726.896	0.004	0.965	53.918	27
20(3 18) - 21(0 21)			41926.604	0.031	0.097	130.567	
7(4 4) - 8(3 5)		42049.780	42049.824	-0.044	0.634	30.301	27
4(3 2) - 5(2 3)		42076.020	42075.986	0.034	0.306	13.686	27
7(4 3) - 8(3 6)		42472.800	42472.736	0.064	0.633	30.301	
25(2 23) - 26(1 26)			42822.160	0.054	0.083	196.631	
1(1 1) - 0(0 0)		43026.600	43026.797	-0.197	1.000	1.435	27
4(3 1) - 5(2 4)		43545.500	43545.540	-0.040	0.304	13.686	
23(5 19) - 24(2 22)			43838.616	0.035	0.196	183.481	
14(3 12) - 15(0 15)			44485.997	0.025	0.094	69.268	
21(3 19) - 22(0 22)			44705.439	0.034	0.094	142.784	
13(3 11) - 12(4 8)		45459.870	45459.643	0.227	1.668	61.075	27
4(0 4) - 3(1 3)		46832.800	46832.851	-0.051	1.761	5.811	27
29(2 28) - 28(3 25)			46933.499	0.080	0.279	251.503	
7(1 6) - 7(0 7)		46980.150	46980.205	-0.055	5.279	17.727	27
16(1 16) - 15(2 13)			47638.243	0.033	0.235	76.701	
10(1 10) - 9(2 7)			48079.145	0.022	0.614	31.694	
16(4 13) - 15(5 10)		48102.770	48102.684	0.086	2.023	93.553	27
22(3 20) - 23(0 23)			48167.750	0.037	0.091	155.565	
13(3 11) - 14(0 14)			48896.710	0.024	0.086	61.075	
19(5 15) - 18(6 12)		49194.000	49193.975	0.025	2.363	132.978	27
19(5 14) - 18(6 13)		49702.400	49702.423	-0.023	2.364	132.995	27
22(6 17) - 21(7 14)		49830.200	49830.515	-0.315	2.699	179.383	17
22(6 16) - 21(7 15)		49950.900	49950.843	0.057	2.699	179.387	17
16(4 12) - 15(5 11)			50099.171	0.011	2.029	93.618	
17(4 14) - 18(1 17)			52020.681	0.026	0.137	103.528	
15(1 15) - 14(2 12)			52101.333	0.032	0.279	67.835	
26(2 24) - 27(1 27)			52171.698	0.059	0.079	211.773	
23(3 21) - 24(0 24)			52228.437	0.042	0.087	168.907	
13(3 10) - 12(4 9)		52372.570	52372.537	0.033	1.701	61.299	27

TABLE 3. Observed and calculated transition frequencies for the ground vibrational state of *trans*-¹²CH₃¹²CH₂¹⁶OH — Continued

Transition		Freq. obs.	Freq. cal.	Uncertainty	Int.	Energy	Ref.
<i>J'</i>	<i>K_a' K_c'</i>	(MHz)	(MHz)	(MHz)	(S)	'state (cm ⁻¹)	
11(1 11)		52670.124	0.025	0.543	37.827	
11(2 10) – 10(53359.400	53359.218	0.182	1.388	41.833	27
8(1 7) – 8(54064.759	0.012	5.381	22.523	
12(3 10) – 13(54641.944	0.023	0.076	53.466	
14(1 14) – 13(54953.271	0.031	0.333	59.515	
12(-1 12) – 11(55323.137	0.027	0.468	44.510	
13(1 13) – 12(56061.616	0.030	0.397	51.739	
10(2 8) – 9(57574.400	57574.699	-0.299	1.431	36.071	27
18(8 11) – 19(57652.990	0.026	1.755	155.652	
18(8 10) – 19(57653.568	0.026	1.755	155.652	
15(7 9) – 16(58279.900	58279.976	-0.076	1.422	112.796	27
15(7 8) – 16(58282.700	58282.632	0.068	1.422	112.796	27
28(2 27) – 27(58778.820	0.068	0.304	235.212	
12(6 7) – 13(58889.539	0.011	1.091	76.936	
12(6 6) – 13(58901.328	0.011	1.091	76.936	
2(1 2) – 1(59297.226	0.005	1.500	2.561	
9(5 5) – 10(59461.837	0.012	0.761	48.073	
9(5 4) – 10(59511.561	0.012	0.761	48.073	
6(4 3) – 7(59943.594	0.013	0.436	26.211	
7(1 6) – 6(59982.342	0.011	1.390	17.727	
6(4 2) – 7(60136.450	0.013	0.436	26.211	
3(3 1) – 4(60214.265	0.014	0.128	11.350	
22(5 18) – 23(60818.987	0.034	0.156	169.966	
3(3 0) – 4(60846.894	0.014	0.128	11.350	
27(2 25) – 28(61138.935	0.065	0.075	227.443	
11(3 9) – 12(61775.990	0.022	0.064	46.441	
25(3 23) – 26(61823.230	0.051	0.081	197.263	
9(1 8) – 9(62407.842	0.014	5.366	27.906	
14(3 12) – 13(62593.444	0.012	1.857	69.268	
16(4 13) – 17(64654.521	0.025	0.110	93.553	
9(2 7) – 9(65484.589	65484.578	0.011	7.394	30.090	b
10(2 8) – 10(65937.717	65937.708	0.009	8.407	36.071	b
8(2 6) – 8(65964.268	0.006	6.317	24.723	
5(0 5) – 4(65997.178	65997.287	-0.109	2.480	8.700	b
17(4 14) – 16(66159.230	66159.201	0.029	2.229	103.528	b
12(2 11) – 11(67140.373	67140.405	-0.032	1.483	48.769	b
7(2 5) – 7(67186.574	67186.577	-0.003	5.237	19.968	b
26(3 24) – 27(67209.221	0.056	0.077	212.274	
11(2 9) – 11(67485.067	67485.049	0.018	9.295	42.664	b
20(5 16) – 19(67490.834	67490.804	0.030	2.574	144.715	b
23(6 18) – 22(68133.981	68134.295	-0.314	2.912	192.873	b
20(5 15) – 19(68328.266	68328.266	0.000	2.576	144.742	b
6(2 4) – 6(68934.899	68934.887	0.012	4.208	15.823	b
17(4 13) – 16(69333.517	0.011	2.240	103.631	
28(2 26) – 29(69735.227	0.072	0.072	243.642	
27(2 26) – 26(70251.305	0.059	0.335	219.462	
12(2 10) – 12(70262.087	70262.072	0.015	10.008	49.869	b
10(3 8) – 11(70336.179	0.021	0.051	40.002	
5(2 3) – 5(70976.836	70976.824	0.012	3.263	12.282	b
10(1 9) – 10(71971.844	71971.780	0.064	5.276	33.871	b
27(3 25) – 28(72899.148	0.062	0.074	227.835	
14(3 11) – 13(73001.994	73001.970	0.024	1.917	69.602	b
4(2 2) – 4(73081.226	73081.215	0.011	2.411	9.341	b
13(2 11) – 13(74380.685	74380.662	0.023	10.516	57.682	b
3(1 3) – 2(74976.055	74976.057	-0.002	2.023	4.249	b
3(2 1) – 3(75036.045	75036.027	0.018	1.637	6.995	b
17(8 10) – 18(75454.987	0.023	1.547	145.132	
17(8 9) – 18(75455.255	0.023	1.547	145.132	
14(7 8) – 15(76071.196	76071.177	-0.019	1.217	104.029	a
14(7 7) – 15(76072.475	76072.388	-0.087	1.217	104.029	a
2(2 0) – 2(76662.495	76662.463	0.032	0.892	5.240	b
11(6 6) – 12(76663.020	76662.862	0.158	0.889	69.923	a
11(6 5) – 12(76668.277	76668.117	0.160	0.889	69.923	a
8(5 4) – 9(77213.738	0.012	0.566	42.815	

TABLE 3. Observed and calculated transition frequencies for the ground vibrational state of *trans*-¹²CH₃¹²CH₂¹⁶OH — Continued

Transition <i>J'</i> <i>K_a'</i> <i>K_c'</i> — <i>J''</i> <i>K_a''</i> <i>K_c''</i>	Freq. obs. (MHz)	Freq. cal. (MHz)	Uncertainty (MHz)	Int. (<i>S</i>)	Energy 'state (cm ⁻¹)	Ref.
8(5 3) — 9(4 6)		77235.098	0.012	0.566	42.815	
5(4 2) — 6(3 3)		77690.497	0.014	0.255	22.707	
5(4 1) — 6(3 4)		77767.794	0.014	0.255	22.707	
29(2 27) — 30(1 30)		77991.419	0.083	0.069	260.370	
28(3 26) — 29(0 29)		78835.263		0.070	0.071	243.945
15(4 12) — 16(1 15)		78927.933	0.024	0.084	84.167	
15(3 13) — 14(4 10)	79367.555	79367.530	0.025	2.031	78.043	b
21(5 17) — 22(2 20)		79532.069	0.033	0.120	157.044	
13(2 12) — 12(3 9)	79762.629	79762.657	-0.028	1.534	56.270	b
11(2 9) — 10(3 8)	79799.196	79799.182	0.014	1.695	42.664	b
14(2 12) — 14(1 13)	79926.068	79926.057	0.011	10.812	66.098	a
2(2 1) — 2(1 2)	80266.218	80266.237	-0.019	0.833	5.239	b
9(3 7) — 10(0 10)		80334.789	0.020	0.037	34.150	
26(2 25) — 25(3 22)		81096.025	0.052	0.374	204.253	
8(1 7) — 7(2 6)	81683.431	81683.426	0.005	1.803	22.523	a
3(2 2) — 3(1 3)	82115.745	82115.709	0.036	1.433	6.988	b
11(1 10) — 11(0 11)	82650.378	82650.311	0.067	5.150	40.413	b
18(4 15) — 17(5 12)	84170.161	84170.115	0.046	2.429	114.094	b
4(2 3) — 4(1 4)	84595.868	84595.823	0.045	1.945	9.320	b
29(3 27) — 30(0 30)		84966.995	0.080	0.069	260.603	
6(0 6) — 5(1 5)	85265.503	85265.509	-0.006	3.280	12.152	a,27
21(5 17) — 20(6 14)	85858.205	85858.164	0.041	2.781	157.044	b,27
30(2 28) — 31(1 31)		85948.184	0.098	0.066	277.629	
15(2 13) — 15(1 14)	86947.306	86947.279	0.027	10.912	75.112	a,27
21(5 16) — 20(6 15)	87200.065	87200.073	-0.008	2.785	157.087	a
5(2 4) — 5(1 5)	87716.102	87716.056	0.046	2.397	12.233	b
18(4 14) — 17(5 13)	89060.815	89060.808	0.007	2.448	114.251	b,27
4(1 4) — 3(0 3)	90117.610	90117.615	-0.005	2.587	6.499	a
14(2 13) — 13(3 10)	91007.730	91007.754	-0.024	1.536	64.334	b
25(2 24) — 24(3 21)		91058.908	0.046	0.423	189.587	
6(2 5) — 6(1 6)	91485.140	91485.123	0.017	2.796	15.726	b
8(3 6) — 9(0 9)		91748.886	0.020	0.025	28.884	
16(8 9) — 17(7 10)	93213.091	93212.866	0.225	1.343	135.198	a,27
16(8 8) — 17(7 11)	93213.091	93212.984	0.107	1.343	135.198	a,27
13(7 7) — 14(6 8)	93812.554	93812.559	-0.005	1.016	95.849	b
13(7 6) — 14(6 9)	93812.855	93813.080	-0.225	1.016	95.849	b
12(1 11) — 12(0 12)	94278.320	94278.256	0.064	5.019	47.525	b,27
10(6 5) — 11(5 6)	94378.564	94378.918	-0.354	0.694	63.496	b
10(6 4) — 11(5 7)	94380.906	94381.086	-0.180	0.694	63.496	b
15(3 12) — 14(4 11)	94477.927	94477.913	0.014	2.135	78.523	b
16(2 14) — 16(1 15)	95444.071	95444.048	0.023	10.853	84.718	a
16(3 14) — 15(4 11)	95650.395	95650.362	0.033	2.182	87.397	b
7(2 6) — 7(1 7)	95909.223	95909.187	0.036	3.146	19.798	b
17(3 14) — 17(2 15)	99524.091	99524.083	0.008	13.592	98.230	a
20(5 16) — 21(2 19)		99816.507	0.033	0.089	144.715	
24(2 23) — 23(3 20)	99896.273	99896.311	-0.038	0.484	175.464	b
18(3 15) — 18(2 16)	99975.883	99975.881	0.002	14.618	109.016	a
16(3 13) — 16(2 14)	100358.958	100358.962	-0.004	12.431	88.066	a
15(2 14) — 14(3 11)	100660.120	100660.166	-0.046	1.490	72.960	b
8(2 7) — 8(1 8)	100990.102	100990.052	0.050	3.447	24.446	b
19(3 16) — 19(2 17)	101873.118	101873.115	0.003	15.451	120.420	a
19(4 16) — 18(5 13)	102075.994	102075.964	0.030	2.620	125.248	b
15(3 12) — 15(2 13)	102283.576	102283.579	-0.003	11.202	78.523	b
12(2 10) — 11(3 9)	102764.355	102764.339	0.016	1.983	49.869	b
9(1 8) — 8(2 7)	103702.902	103702.896	0.006	2.276	27.906	a
22(5 18) — 21(6 15)	104279.740	104279.636	0.104	2.985	169.966	a
7(0 7) — 6(1 6)	104487.260	104487.260	0.000	4.158	16.160	a
7(3 5) — 8(0 8)		104510.385	0.020	0.015	24.205	
5(1 5) — 4(0 4)	104808.632	104808.641	-0.009	3.205	9.308	a
14(3 11) — 14(2 12)	105064.311	105064.322	-0.011	9.972	69.602	b
20(3 17) — 20(2 18)	105337.369	105337.373	-0.004	16.052	132.440	a
17(2 15) — 17(1 16)	105355.636	105355.610	0.026	10.682	94.910	a
22(5 17) — 21(6 16)	106375.782	106375.806	-0.024	2.991	170.034	a
13(1 12) — 13(0 13)	106649.479	106649.425	0.054	4.904	55.201	b

TABLE 3. Observed and calculated transition frequencies for the ground vibrational state of *trans*-¹²CH₃¹²CH₂¹⁶OH — Continued

Transition		Freq. obs. (MHz)	Freq. cal. (MHz)	Uncertainty (MHz)	Int. (S)	Energy 'state (cm ⁻¹)	Ref.
J'	K _a ' K _c ' J'' K _a '' K _c ''						
9(2 8)– 9(1 9)		106723.558	106723.508	0.050	3.702	29.670	b
23(2 22)– 22(3 19)			107381.490	0.037	0.559	161.884	
13(3 10)– 13(2 11)		108438.579	108438.592	-0.013	8.795	61.299	b
16(2 15)– 15(3 12)		108524.526	108524.536	-0.010	1.403	82.143	b
19(4 15)– 18(5 14)		109394.865	109394.882	-0.017	2.652	125.482	b
21(3 18)– 21(2 19)			110452.280	0.014	16.406	145.070	
15(8 8)– 16(7 9)		110931.121	110931.112	0.009	1.144	125.849	a
15(8 7)– 16(7 10)		110931.121	110931.162	-0.041	1.144	125.849	a
17(3 15)– 16(4 12)		111287.163	111287.131	0.032	2.305	97.330	b
12(7 6)– 13(6 7)		111510.277	111510.165	0.112	0.822	88.254	a
12(7 5)– 13(6 8)		111510.277	111510.374	-0.097	0.822	88.254	a
13(4 10)– 14(1 13)			111988.409	0.022	0.041	67.167	
9(6 4)– 10(5 5)		112046.635	112046.569	0.066	0.510	57.655	a
9(6 3)– 10(5 6)		112047.555	112047.384	0.171	0.510	57.655	a
12(3 9)– 12(2 10)		112129.544	112129.564	-0.020	7.707	53.609	b
6(5 2)– 7(4 3)		112523.049	112523.388	-0.339	0.219	34.054	b
6(5 1)– 7(4 4)		112526.378	112526.135	0.243	0.219	34.054	a
2(2 1)– 1(1 0)		112807.174	112807.142	0.032	1.500	5.239	b,27
10(2 9)– 10(1 10)		113098.078	113098.026	0.052	3.915	35.466	b
22(2 21)– 21(3 18)		113308.991	113308.951	0.040	0.649	148.849	b
2(2 0)– 1(1 1)		114064.943	114064.893	0.050	1.465	5.240	b,27
17(2 16)– 16(3 13)		114443.972	114443.974	-0.002	1.286	91.883	b
11(3 8)– 11(2 9)		115866.101	115866.141	-0.040	6.721	46.529	b
18(2 16)– 18(1 17)		116556.704	116556.693	0.011	10.452	105.681	a
16(3 13)– 15(4 12)		116875.092	116875.077	0.015	2.358	88.066	b
22(3 19)– 22(2 20)		117258.405	117258.403	0.002	16.525	158.302	a
21(2 20)– 20(3 17)		117498.197	117498.160	0.037	0.755	136.359	b
18(2 17)– 17(3 14)			118314.755	0.024	1.151	102.177	
6(3 4)– 7(0 7)			118500.582	0.022	0.008	20.113	
6(1 6)– 5(0 5)			119165.009	0.009	3.891	12.675	
10(3 7)– 10(2 8)		119404.930	119404.875	0.055	5.836	40.053	27
14(1 13)– 14(0 14)		119539.110	119539.082	0.028	4.813	63.431	27
20(2 19)– 19(3 16)			119798.107	0.028	0.877	124.416	
20(4 17)– 19(5 14)			119800.098	0.013	2.799	136.991	
19(2 18)– 18(3 15)			120093.804	0.026	1.011	113.022	
11(2 10)– 11(1 11)			120093.969	0.013	4.088	41.833	
19(5 15)– 20(2 18)			121464.206	0.033	0.064	132.978	
9(3 6)– 9(2 7)		122550.649	122550.677	-0.028	5.039	34.178	b
23(5 19)– 22(6 16)			122729.835	0.019	3.183	183.481	
8(0 8)– 7(1 7)			123527.855	0.008	5.105	20.719	
8(3 5)– 8(2 6)		125173.193	125173.182	0.011	4.308	28.898	b,27
23(3 20)– 23(2 21)		125744.574	125744.574	0.000	16.445	172.132	a
23(5 18)– 22(6 17)		125927.302	125927.341	-0.039	3.194	183.584	a,27
10(1 9)– 9(2 8)		125947.361	125947.341	0.020	2.817	33.871	a,27
18(3 16)– 17(4 13)		126099.740	126099.703	0.037	2.394	107.837	b,27
13(2 11)– 12(3 10)		126387.955	126388.144	-0.189	2.304	57.682	a
7(3 4)– 7(2 5)		127215.151	127215.146	0.005	3.622	24.212	b,27
12(2 11)– 12(1 12)		127683.444	127683.410	0.034	4.227	48.769	b
14(8 7)– 15(7 8)		128613.976	128613.922	0.054	0.950	117.086	a
14(8 6)– 15(7 9)		128613.976	128613.942	0.034	0.950	117.086	a
6(3 3)– 6(2 4)		128689.666	128689.646	0.020	2.963	20.116	b
19(2 17)– 19(1 18)		128863.083	128863.096	-0.013	10.207	117.022	a
3(2 2)– 2(1 1)		129077.648	129077.620	0.028	1.667	6.988	b
11(7 5)– 12(6 6)		129169.630	129169.529	0.101	0.637	81.244	a
11(7 4)– 12(6 7)		129169.630	129169.606	0.024	0.637	81.244	a
5(3 2)– 5(2 3)		129665.731	129665.696	0.035	2.308	16.607	b
8(6 3)– 9(5 4)		129673.719	129673.589	0.130	0.341	52.399	a
8(6 2)– 9(5 5)		129674.046	129673.861	0.185	0.341	52.399	a
5(5 1)– 6(4 2)			130108.831	0.014	0.085	30.551	
5(5 0)– 6(4 3)			130109.581	0.014	0.085	30.551	
4(3 1)– 4(2 2)			130246.225	0.012	1.635	13.686	
12(4 9)– 13(1 12)			130446.718	0.021	0.026	59.552	
20(4 16)– 19(5 15)		130458.049	130458.009	0.040	2.854	137.330	a
3(3 0)– 3(2 1)		130545.153	130544.951	0.202	0.901	11.350	a

TABLE 3. Observed and calculated transition frequencies for the ground vibrational state of *trans*-¹²CH₃¹²CH₂¹⁶OH — Continued

Transition		Freq. obs.	Freq. cal.	Uncertainty	Int.	Energy	Ref.
<i>J'</i>	<i>K_a' K_c'</i>	(MHz)	(MHz)	(MHz)	(S)	'state (cm ⁻¹)	
<i>J''</i>	<i>K_a'' K_c''</i>						
3(3 1)– 3(2 2)		130755.300	130755.419	-0.119	0.900	11.350	b
4(3 2)– 4(2 3)		130871.493	130871.477	0.016	1.630	13.686	b
5(3 3)– 5(2 4)		131103.040	131103.014	0.026	2.292	16.607	b
25(4 21)– 25(3 22)		131441.812	131441.827	-0.015	19.912	205.933	a
6(3 4)– 6(2 5)		131502.758	131502.719	0.039	2.921	20.113	b
24(4 20)– 24(3 21)		132118.876	132118.869	0.007	18.747	190.957	a
7(3 5)– 7(2 6)		132129.069	132129.052	0.017	3.531	24.205	a
26(4 22)– 26(3 23)		132373.040	132373.062	-0.022	20.874	221.534	a
15(1 14)– 15(0 15)		132727.661	132727.641	0.020	4.748	72.211	b
3(2 1)– 2(1 2)		132935.154	132935.133	0.021	1.550	6.995	b
8(3 6)– 8(2 7)		133043.918	133043.939	-0.021	4.125	28.884	b
7(1 7)– 6(0 6)		133323.455	133323.470	-0.015	4.650	16.599	a
5(3 3)– 6(0 6)			133553.561	0.023	0.003	16.607	
23(4 19)– 23(3 20)		134219.627	134219.611	0.016	17.447	176.609	a
9(3 7)– 9(2 8)		134310.371	134310.350	0.021	4.703	34.150	b
27(4 23)– 27(3 24)		135051.366	135051.423	-0.057	21.585	237.756	a
13(2 12)– 13(1 13)		135830.641	135830.605	0.036	4.337	56.270	b
24(3 21)– 24(2 22)		135839.262	135839.227	0.035	16.219	186.550	a
10(3 8)– 10(2 9)		135989.916	135989.902	0.014	5.262	40.002	b
21(4 18)– 20(5 15)		137246.807	137246.773	0.034	2.963	149.320	a
22(4 18)– 22(3 19)		137514.812	137514.754	0.058	16.084	162.889	a
11(3 9)– 11(2 10)		138140.624	138140.600	0.024	5.796	46.441	b
28(4 24)– 28(3 25)		139569.485	139569.556	-0.071	22.023	254.593	a
19(3 17)– 18(4 14)		139888.278	139888.274	0.004	2.441	118.917	a
17(3 14)– 16(4 13)		140225.169	140225.172	-0.003	2.591	98.230	b
12(3 10)– 12(2 11)		140814.810	140814.805	0.005	6.299	53.466	b
21(4 17)– 21(3 18)		141735.490	141735.441	0.049	14.727	149.797	a
20(2 18)– 20(1 19)		142046.310	142046.318	-0.008	9.979	128.926	b
9(0 9)– 8(1 8)		142285.054	142285.106	-0.052	6.103	25.824	a
13(3 11)– 13(2 12)		144057.496	144057.487	0.009	6.766	61.075	b
18(5 14)– 19(2 17)			144234.246	0.033	0.045	121.833	
14(2 13)– 14(1 14)		144493.107	144493.075	0.032	4.421	64.334	b
4(2 3)– 3(1 2)		144734.098	144734.084	0.014	1.886	9.320	b
24(5 19)– 23(6 18)		145941.945	145941.882	0.063	3.392	197.741	a
29(4 25)– 29(3 26)		145970.947	145971.025	-0.078	22.191	272.039	a
16(1 15)– 16(0 16)		146022.067	146022.068	-0.001	4.706	81.534	b
13(8 6)– 14(7 7)		146265.257	146265.225	0.032	0.765	108.908	a
13(8 5)– 14(7 8)		146265.257	146265.232	0.025	0.765	108.908	a
20(4 16)– 20(3 17)		146584.895	146584.841	0.054	13.431	137.330	a
10(7 4)– 11(6 5)		146795.873	146795.745	0.128	0.464	74.820	a
10(7 3)– 11(6 6)		146795.873	146795.771	0.102	0.464	74.820	a
7(6 2)– 8(5 3)		147267.095	147266.876	0.219	0.192	47.727	a
7(6 1)– 8(5 4)		147267.095	147266.953	0.142	0.192	47.727	a
25(3 22)– 25(2 23)		147406.345	147406.268	0.077	15.903	201.548	a
8(1 8)– 7(0 7)		147427.463	147427.484	-0.021	5.483	21.078	a
14(3 12)– 14(2 13)		147904.805	147904.793	0.012	7.191	69.268	b
11(1 10)– 10(2 9)		148304.057	148304.035	0.022	3.435	40.413	a
4(3 2)– 5(0 5)			149470.012	0.025	0.001	13.686	
11(4 8)– 12(1 11)			149907.829	0.021	0.016	52.526	
14(2 12)– 13(3 11)		150568.422	150568.429	-0.007	2.666	66.098	a
19(4 15)– 19(3 16)		151756.036	151756.012	0.024	12.230	125.482	a
21(4 17)– 20(5 16)		152371.083	152371.214	-0.131	3.054	149.797	a
15(3 13)– 15(2 14)		152382.962	152382.944	0.018	7.573	78.043	b
20(3 18)– 19(4 15)		152435.789	152435.727	0.062	2.442	130.567	a
4(2 2)– 3(1 3)		152656.891	152656.863	0.028	1.625	9.341	a
15(2 14)– 15(1 15)		153623.149	153623.156	-0.007	4.486	72.960	b
22(4 19)– 21(5 16)			154299.445	0.016	3.107	162.234	
21(2 19)– 21(1 20)		153854.475	153854.463	0.012	9.787	141.385	a
18(4 14)– 18(3 15)		156953.760	156953.760	0.000	11.139	114.251	a
16(3 14)– 16(2 15)		157507.479	157507.463	0.016	7.909	87.397	b
17(1 16)– 17(0 17)		159271.184	159271.205	-0.021	4.681	91.396	b
5(2 4)– 4(1 3)		159781.897	159781.900	-0.003	2.138	12.233	a
26(3 23)– 26(2 24)		160248.962	160248.819	0.143	15.555	217.118	a
10(0 10)– 9(1 9)		160699.059	160699.069	-0.010	7.134	31.470	a

TABLE 3. Observed and calculated transition frequencies for the ground vibrational state of *trans*-¹²CH₃¹²CH₂¹⁶OH — Continued

Transition		Freq. obs. (MHz)	Freq. cal. (MHz)	Uncertainty (MHz)	Int. (S)	Energy 'state (cm ⁻¹)	Ref.
J' K _a ' K _c '	J'' K _a '' K _c ''						
9(1 9) – 8(0 8)		161609.018	161609.048	-0.030	6.381	26.110	
17(4 13) – 17(3 14)		161917.203	161917.222	-0.019	10.157	103.631	b
24(6 19) – 25(3 22)			162091.903	0.049	0.060	206.955	
16(2 15) – 16(1 16)		163169.861	163169.872	-0.011	4.535	82.143	b
17(3 15) – 17(2 16)		163282.790	163282.773	0.017	8.199	97.330	b
21(3 19) – 20(4 16)		163515.766	163515.719	0.047	2.394	142.784	a
12(8 5) – 13(7 6)		163888.752	163888.699	0.053	0.589	101.315	a
12(8 4) – 13(7 7)		163888.752	163888.701	0.051	0.589	101.315	a
9(7 3) – 10(6 4)		164393.515	164393.508	0.007	0.307	68.980	a
9(7 2) – 10(6 5)		164393.515	164393.516	-0.001	0.307	68.980	a
18(3 15) – 17(4 14)		164511.879	164511.893	-0.014	2.841	109.016	a
6(6 1) – 7(5 2)		164832.842	164832.591	0.251	0.073	43.641	a
6(6 0) – 7(5 3)		164832.842	164832.609	0.233	0.073	43.641	a
3(3 1) – 4(0 4)			166038.277	0.026	0.000	11.350	
16(4 12) – 16(3 13)		166439.597	166439.616	-0.019	9.270	93.618	b
25(5 20) – 24(6 19)		166522.196	166522.084	0.112	3.586	212.510	a
17(5 13) – 18(2 16)			167868.834	0.032	0.031	111.280	
18(3 16) – 18(2 17)		169702.194	169702.171	0.023	8.444	107.837	a
22(2 20) – 22(1 21)		170035.912	170035.907	0.005	9.640	154.391	b
10(4 7) – 11(1 10)			170136.923	0.022	0.009	46.088	
15(4 11) – 15(3 12)		170381.606	170381.637	-0.031	8.460	84.207	b
12(1 11) – 11(2 10)		170642.867	170642.867	0.000	4.138	47.525	a
23(4 20) – 22(5 17)		170819.392	170819.369	0.023	3.227	175.732	a
18(1 17) – 18(0 18)		172372.220	172372.253	-0.033	4.668	101.793	b
22(3 20) – 21(4 17)		172905.077	172905.021	0.056	2.298	155.565	a
17(2 16) – 17(1 17)		173080.903	173080.921	-0.018	4.572	91.883	b
5(2 3) – 4(1 4)		173391.333	173391.313	0.020	1.655	12.282	b
27(3 24) – 27(2 25)		174121.820	174121.592	0.228	15.217	233.251	a
6(2 5) – 5(1 4)		174232.909	174232.930	-0.021	2.420	15.726	a
15(2 13) – 14(3 12)		175188.995	175188.923	0.072	3.080	75.112	a
22(4 18) – 21(5 17)		175240.955	175241.088	-0.133	3.255	162.889	a
10(1 10) – 9(0 9)		175971.482	175971.566	-0.084	7.331	31.694	a
13(4 9) – 13(3 10)		176319.000	176319.103	-0.103	6.998	67.180	a
19(3 17) – 19(2 18)		176748.257	176748.231	0.026	8.648	118.917	a
12(4 8) – 12(3 9)		178360.461	178360.501	-0.040	6.318	59.559	a
11(0 11) – 10(1 10)		178751.724	178751.750	-0.026	8.181	37.656	a
11(4 7) – 11(3 8)		179879.792	179879.819	-0.027	5.658	52.529	a
29(3 27) – 28(4 24)			180150.774	0.078	1.076	260.603	
23(3 21) – 22(4 18)		180399.524	180399.481	0.043	2.159	168.907	a
14(9 6) – 15(8 7)			180949.678	0.023	0.714	131.885	
14(9 5) – 15(8 8)			180949.678	0.023	0.714	131.885	
10(4 6) – 10(3 7)		180970.651	180970.678	-0.027	5.010	46.090	a
11(8 4) – 12(7 5)			181487.788	0.016	0.426	94.308	
11(8 3) – 12(7 6)			181487.788	0.016	0.426	94.308	
9(4 5) – 9(3 6)		181726.121	181726.177	-0.056	4.369	40.240	a
8(7 2) – 9(6 3)			181967.141	0.019	0.171	63.725	
8(7 1) – 9(6 4)			181967.143	0.019	0.171	63.725	
8(4 4) – 8(3 5)		182230.045	182230.018	0.027	3.727	34.977	b
11(4 8) – 11(3 9)		182410.074	182410.096	-0.022	5.625	52.526	b
10(4 7) – 10(3 8)		182451.030	182451.056	-0.026	4.994	46.088	b
12(4 9) – 12(3 10)		182454.172	182454.199	-0.027	6.258	59.552	b
9(4 6) – 9(3 7)		182538.226	182538.240	-0.014	4.361	40.239	b
7(4 3) – 7(3 4)		182552.442	182552.284	0.158	3.078	30.301	a
13(4 10) – 13(3 11)		182630.753	182630.782	-0.029	6.890	67.167	b
8(4 5) – 8(3 6)		182641.951	182641.976	-0.025	3.724	34.977	b
7(4 4) – 7(3 5)		182741.594	182741.648	-0.054	3.077	30.301	b
6(4 2) – 6(3 3)		182748.752	182748.543	0.209	2.410	26.211	a
6(4 3) – 6(3 4)		182824.767	182824.940	-0.173	2.409	26.211	b
5(4 1) – 5(3 2)		182861.206	182860.923	0.283	1.703	22.707	b
5(4 2) – 5(3 3)		182886.782	182886.553	0.229	1.703	22.707	b
4(4 0) – 4(3 1)		182920.438	182920.119	0.319	0.925	19.788	a
4(4 1) – 4(3 2)		182926.336	182926.557	-0.221	0.925	19.788	b
14(4 11) – 14(3 12)		182994.578	182994.589	-0.011	7.520	75.372	b
3(3 1) – 2(2 0)		183170.436	183170.576	-0.140	2.485	11.350	b

TABLE 3. Observed and calculated transition frequencies for the ground vibrational state of *trans*-¹³CH₃¹²CH₂¹⁶OH — Continued

Transition		Freq. obs.	Freq. cal.	Uncertainty	Int.	Energy	Ref.
<i>J'</i>	<i>K_a' K_c' J''</i>	(MHz)	(MHz)	(MHz)	(<i>S</i>)	'state (cm ⁻¹)	
3(3 0) - 2(183214.030	183213.848	0.182	2.485	11.350	a
18(2 17) - 18(183304.546	183304.584	-0.038	4.599	102.177	b
15(4 12) - 15(183605.574	183605.877	-0.303	8.145	84.167	a
23(2 21) - 23(184361.991	184361.908	0.083	9.534	167.937	a
20(3 18) - 20(184393.717	184393.632	0.085	8.815	130.567	a
16(4 13) - 16(184528.228	184528.183	0.045	8.761	93.553	a
19(1 18) - 19(185268.167	185268.285	-0.118	4.663	112.724	a
28(3 26) - 27(185543.408	0.061	1.234	243.945	
17(4 14) - 17(185825.858	0.013	9.361	103.528	
24(3 22) - 23(185831.393	0.030	1.989	182.807	
24(4 21) - 23(186644.765	0.020	3.317	189.809	
18(4 15) - 18(187561.546	0.013	9.940	114.094	
7(2 6) - 6(188107.573	0.012	2.735	19.798	
28(3 25) - 28(188750.280	0.032	14.921	249.938	
27(3 25) - 26(188901.640	0.049	1.411	227.835	
25(3 23) - 24(189084.772	0.035	1.799	197.264	
23(6 18) - 24(189561.052	0.043	0.044	192.873	
19(3 16) - 18(189673.501	0.019	3.117	120.420	
19(4 16) - 19(189793.754	0.014	10.491	125.248	
26(3 24) - 25(190105.082	0.041	1.602	212.274	
11(1 11) - 10(190579.612	0.011	8.317	37.827	
26(5 21) - 26(190674.898	0.034	16.785	227.894	
9(4 6) - 10(190901.250	0.023	0.005	40.239	
16(5 12) - 17(192107.788	0.031	0.020	101.318	
20(4 17) - 20(192574.664	0.015	11.008	136.991	
21(3 19) - 21(192602.400	0.014	8.948	142.784	
13(1 12) - 12(192822.286	0.013	4.929	55.201	
19(2 18) - 19(193791.351	193791.411	-0.060	4.619	113.022	a
6(2 4) - 5(195325.481	0.012	.630	15.823	
21(4 18) - 21(195948.255	0.015	11.486	149.320	
12(0 12) - 11(196458.580	0.010	9.233	44.381	
25(5 20) - 25(197172.160	0.028	15.616	212.510	
20(1 19) - 20(197939.372	0.021	4.662	124.188	
16(10 6) - 17(197975.287	0.073	0.840	166.526	
16(10 7) - 17(197975.287	0.073	0.840	166.526	
13(9 5) - 14(198547.523	0.019	0.547	123.709	
13(9 4) - 14(198547.523	0.019	0.547	123.709	
24(2 22) - 24(198644.410	0.021	9.463	182.019	
10(8 3) - 11(199065.704	0.018	0.279	87.884	
10(8 2) - 11(199065.704	0.018	0.279	87.884	
23(4 19) - 22(199145.199	0.022	3.460	176.609	
7(7 1) - 8(199520.617	0.022	0.064	59.054	
7(7 0) - 8(199520.617	0.022	0.064	59.054	
22(4 19) - 22(199948.815	0.016	11.920	162.234	
16(2 14) - 15(200121.992	0.017	3.555	84.718	
4(3 2) - 3(200569.534	0.013	2.579	13.686	
4(3 1) - 3(200787.380	0.013	2.577	13.686	
22(3 20) - 22(201331.510	0.015	9.053	155.565	
8(2 7) - 7(201437.332	0.012	3.088	24.446	
25(4 22) - 24(201590.968	0.024	3.369	204.465	
24(5 19) - 24(203384.064	0.023	14.562	197.741	
29(3 26) - 29(203854.869	0.038	14.680	267.170	
20(2 19) - 20(204495.550	0.021	4.634	124.416	
23(4 20) - 23(204599.863	0.016	12.309	175.732	
12(1 12) - 11(205458.497	0.011	9.325	44.510	
23(5 18) - 23(209100.261	209100.137	0.124	13.608	183.584	
24(4 21) - 24(209913.509	0.017	12.650	189.809	
21(1 20) - 21(210391.112	210391.175	-0.063	4.663	136.186	b
23(3 21) - 23(210532.832	210532.745	0.087	9.135	168.907	a
8(4 5) - 9(211983.020	0.025	0.002	34.977	
25(2 23) - 25(212746.107	212746.056	0.051	9.420	196.631	a
13(0 13) - 12(213856.261	213856.270	-0.009	10.282	51.643	a
22(5 17) - 22(214180.117	214179.975	0.142	12.736	170.034	a
9(2 8) - 8(214267.743	214267.797	-0.054	3.486	29.670	a

TABLE 3. Observed and calculated transition frequencies for the ground vibrational state of *trans*-¹²CH₃¹²CH₂¹⁶OH — Continued

Transition		Freq. obs.	Freq. cal.	Uncertainty	Int.	Energy	Ref.
<i>J'</i>	<i>K_a' K_c' J''</i>	(MHz)	(MHz)	(MHz)	(S)	'state (cm ⁻¹)	
14(1 13) – 13(214699.879	214699.859	0.020	5.805	63.431	a
21(2 20) – 21(215375.642	215375.682	-0.040	4.646	136.359	b
26(4 23) – 25(215452.238	215452.202	0.036	3.379	219.696	a
20(3 17) – 19(215610.762	0.020	3.428	132.440	
25(4 22) – 25(215890.440	215890.261	0.179	12.944	204.465	a
12(9 4) – 13(216127.000	216126.776	0.224	0.393	116.117	a
12(9 3) – 13(216127.000	216126.776	0.224	0.393	116.117	a
9(8 2) – 10(216625.420	216625.442	-0.022	0.154	82.045	a
9(8 1) – 10(216625.420	216625.442	-0.022	0.154	82.045	a
15(5 11) – 16(216699.408	0.030	0.013	84.718	
22(6 17) – 23(217392.407	0.039	0.032	172.132	
5(3 3) – 4(217803.689	217803.699	-0.010	2.714	16.607	a
5(3 2) – 4(218461.226	218461.187	0.039	2.706	16.607	a
21(5 16) – 21(218554.499	218554.391	0.108	11.926	157.087	a
7(2 5) – 6(218654.081	218654.042	0.039	1.550	19.968	a
24(3 22) – 24(220154.784	220154.693	0.091	9.198	182.807	a
13(1 13) – 12(220601.927	220601.945	-0.018	10.344	51.739	a
20(5 15) – 20(222217.285	222217.201	0.084	11.164	144.742	a
26(4 23) – 26(222519.499	222519.281	0.218	13.193	219.696	a
22(1 21) – 22(222644.166	222644.229	-0.063	4.665	148.719	b
24(4 20) – 23(224119.273	224119.480	-0.207	3.676	190.957	a
19(5 14) – 19(225210.356	225210.293	0.063	10.435	132.995	a
17(2 15) – 16(225229.250	225229.272	-0.022	4.102	94.910	a
22(2 21) – 22(226395.490	226395.538	-0.048	4.654	148.849	b
26(2 24) – 26(226581.339	226581.326	0.013	9.394	211.773	a
10(2 9) – 9(226661.701	226661.750	-0.049	3.938	35.466	a
18(5 13) – 18(227606.079	227606.064	0.015	9.732	121.843	a
27(4 24) – 26(228005.820	228005.817	0.003	3.342	235.499	a
17(5 12) – 17(229491.131	229491.134	-0.003	9.048	111.286	a
27(4 24) – 27(229779.303	229779.075	0.228	13.400	235.499	a
25(3 23) – 25(230144.820	230144.733	0.087	9.245	197.264	a
16(5 11) – 16(230953.778	230953.788	-0.010	8.379	101.321	a
14(0 14) – 13(230991.374	230991.382	-0.008	11.325	59.444	a
21(5 17) – 21(231558.549	231558.511	0.038	11.670	157.044	a
20(5 16) – 20(231560.901	231560.878	0.023	11.003	144.715	a
19(5 15) – 19(231737.606	231737.595	0.011	10.337	132.978	a
22(5 18) – 22(231790.000	231789.994	0.006	12.332	169.966	a
18(5 14) – 18(232034.630	232034.632	-0.002	9.673	121.833	a
15(5 10) – 15(232075.832	232075.861	-0.029	7.721	91.948	a
23(5 19) – 23(232318.499	232318.457	0.042	12.985	183.481	a
17(5 13) – 17(232404.808	232404.845	-0.037	9.013	111.280	a
16(5 12) – 16(232808.832	232808.877	-0.045	8.359	101.318	a
14(5 9) – 14(232928.499	232928.546	-0.047	7.072	83.165	a
14(10 5) – 15(233147.883	233147.983	-0.100	0.511	148.423	a
14(10 4) – 15(233147.883	233147.983	-0.100	0.511	148.423	a
7(4 4) – 8(233187.274	0.027	0.001	30.301	
24(5 20) – 24(233208.521	233208.512	0.009	13.623	197.588	a
15(5 11) – 15(233215.475	233215.523	-0.048	7.710	91.946	a
13(5 8) – 13(233571.024	233571.071	-0.047	6.430	74.971	a
14(5 10) – 14(233601.523	233601.578	-0.055	7.066	83.164	a
13(5 9) – 13(233951.119	233951.252	-0.133	6.427	74.971	a
12(5 7) – 12(234051.119	234051.162	-0.043	5.790	67.366	a
8(8 1) – 9(234169.691	234169.777	-0.086	0.057	76.791	a
8(8 0) – 9(234169.691	234169.777	-0.086	0.057	76.791	a
12(5 8) – 12(234255.161	234255.255	-0.094	5.789	67.366	b
11(5 6) – 11(234406.451	234406.436	0.015	5.151	60.348	a
11(5 7) – 11(234509.565	234509.671	-0.106	5.151	60.348	b
25(5 21) – 25(234523.893	234523.936	-0.043	14.241	212.288	a
10(5 5) – 10(234666.273	234666.132	0.141	4.508	53.918	a
10(5 6) – 10(234714.571	234714.773	-0.202	4.508	53.918	b
23(1 22) – 23(234725.600	234725.664	-0.064	4.668	161.788	b
6(3 4) – 5(234758.820	234758.825	-0.005	2.864	20.113	a
9(5 4) – 9(234853.026	234852.837	0.189	3.856	48.073	a
9(5 5) – 9(234873.612	234873.848	-0.236	3.856	48.073	b

TABLE 3. Observed and calculated transition frequencies for the ground vibrational state of *trans*-¹³CH₃¹²CH₂¹⁶OH — Continued

Transition <i>J'</i> <i>K'₁' K'₂'</i> <i>J''</i> <i>K₁'' K₂''</i>	Freq. obs. (MHz)	Freq. cal. (MHz)	Uncertainty (MHz)	Int. (<i>S</i>)	Energy 'state (cm ⁻¹)	Ref.
8(5 3)– 8(4 4)	234984.238	234984.017	0.221	3.188	42.815	a
8(5 4)– 8(4 5)	234991.905	234992.150	-0.245	3.188	42.815	b
7(5 2)– 7(4 3)	235073.491	235073.276	0.215	2.493	38.142	a
7(5 3)– 7(4 4)	235075.767	235076.002	-0.235	2.493	38.142	b
6(5 1)– 6(4 2)	235131.505	235131.332	0.173	1.753	34.054	a
6(5 2)– 6(4 3)	235132.356	235132.079	0.277	1.753	34.054	a
5(5 0)– 5(4 1)	235166.636	235166.727	-0.091	0.941	30.551	a
5(5 1)– 5(4 2)	235166.636	235166.877	-0.241	0.941	30.551	a
14(1 14)– 13(0 13)	235983.333	235983.359	-0.026	11.366	59.515	a
15(1 14)– 14(2 13)	236146.428	236146.437	-0.009	6.757	72.211	a
6(3 3)– 5(2 4)	236299.071	236299.070	0.001	2.843	20.116	a
26(5 22)– 26(4 23)	236325.166	236325.335	-0.169	14.833	227.579	a
23(2 22)– 23(1 23)	237524.119	237524.058	0.061	4.661	161.884	a
28(4 25)– 28(3 26)	237638.792	237638.597	0.195	13.569	251.872	a
27(5 23)– 27(4 24)	238667.525	238667.931	-0.406	15.391	243.461	a
11(2 10)– 10(1 9)	238701.760	238701.801	-0.041	4.453	41.833	a
28(4 25)– 27(5 22)	239019.855	239019.851	0.004	3.254	251.872	a
27(2 25)– 27(1 26)	240110.238	240110.207	0.031	9.381	227.443	a
26(3 24)– 26(2 25)	240450.950	240450.884	0.066	9.281	212.274	a
14(5 10)– 15(2 13)		241407.244	0.028	0.008	83.164	
21(3 18)– 20(4 17)	242196.547	242196.652	-0.105	3.783	145.070	a
8(2 6)– 7(1 7)	243556.939	243556.881	0.058	1.425	24.723	a
21(6 16)– 22(3 19)		245318.923	0.037	0.023	166.485	
13(10 4)– 14(9 5)	250711.624	250711.680	-0.056	0.365	140.248	a
13(10 3)– 14(9 6)	250711.624	250711.680	-0.056	0.365	140.248	a
27(3 25)– 27(2 26)	251023.404	251023.397	0.007	9.308	227.835	a
10(9 2)– 11(8 3)	251238.602	251238.649	-0.047	0.140	102.688	a
10(9 1)– 11(8 4)	251238.602	251238.649	-0.047	0.140	102.688	a
7(3 5)– 6(2 4)	251301.713	251301.738	-0.025	3.019	24.205	a
15(1 15)– 14(0 14)	251566.455	251566.471	-0.016	12.389	67.835	a
4(4 1)– 3(3 0)	252951.382	252951.140	0.242	3.486	19.788	a
4(4 0)– 3(3 1)	252952.404	252952.079	0.325	3.486	19.788	a
28(2 26)– 28(1 27)		253327.459	0.029	9.376	243.642	
6(4 3)– 7(1 6)		254345.317	0.029	0.000	26.211	
7(3 4)– 6(2 5)		254384.065	0.012	2.971	24.212	
16(1 15)– 15(2 14)		257060.888	0.011	7.769	81.534	
25(1 24)– 25(0 25)	258484.657	258484.678	-0.021	4.674	189.535	b
25(2 24)– 25(1 25)	260007.728	260007.746	-0.018	4.671	189.587	b
28(3 26)– 28(2 27)	261815.990	261816.010	-0.020	9.328	243.945	a
13(2 12)– 12(1 11)	262154.267	262154.293	-0.026	5.703	56.270	a
31(4 28)– 31(3 29)	264394.089	264394.187	-0.098	13.895	304.373	a
33(3 30)– 33(2 31)	264426.465	264426.338	0.127	14.219	341.424	a
16(0 16)– 15(1 15)	264662.000	264661.976	0.024	13.392	76.664	a
13(5 9)– 14(2 12)		266013.605	0.027	0.005	74.971	
29(2 27)– 29(1 28)	266250.737	266250.892	-0.155	9.374	260.370	a
27(6 21)– 27(5 22)	266971.905	266971.973	-0.068	15.429	252.804	a
8(3 6)– 7(2 5)	267294.701	267294.695	0.006	3.175	28.884	a
16(1 16)– 15(0 15)	267313.190	267313.163	0.027	13.411	76.701	a
12(10 3)– 13(9 4)	268262.584	268262.631	-0.047	0.236	132.657	a
12(10 2)– 13(9 5)	268262.584	268262.631	-0.047	0.236	132.657	a
9(9 1)– 10(8 2)	268775.513	268775.478	0.035	0.051	96.850	a
9(9 0)– 10(8 3)	268775.513	268775.478	0.035	0.051	96.850	a
22(3 19)– 21(4 18)	269284.737	269284.845	-0.108	4.192	158.302	a
9(2 7)– 8(1 8)	270177.618	270177.527	0.091	1.271	30.090	a
26(1 25)– 26(0 26)	270211.327	270211.313	0.014	4.676	204.215	b
5(4 2)– 4(3 1)	270443.757	270444.027	-0.270	3.558	22.707	b
5(4 1)– 4(3 2)	270450.945	270450.632	0.313	3.557	22.707	a
26(6 20)– 26(5 21)	270787.572	270787.343	0.229	14.659	236.926	a
26(2 25)– 26(1 26)	271324.455	271324.452	0.003	4.674	204.253	b
29(3 27)– 29(2 28)	272786.624	272786.831	-0.207	9.343	260.603	a
8(3 5)– 7(2 6)	272820.921	272820.876	0.045	3.080	8.898	a
20(6 15)– 21(3 18)		273089.758	0.036	0.016	154.179	
14(2 13)– 13(1 12)	273827.000	273827.009	-0.009	6.448	64.334	a
32(4 29)– 32(3 30)	274206.673	274207.105	-0.432	13.959	322.992	a

TABLE 3. Observed and calculated transition frequencies for the ground vibrational state of *trans*-¹²CH₃¹²CH₂¹⁶OH—Continued

Transition		Freq. obs.	Freq. cal.	Uncertainty	Int.	Energy	Ref.
J' K _a ' K _c '	J'' K _{a}'' K_{c}''}}	(MHz)	(MHz)	(MHz)	(S)	'state (cm ⁻¹)	
5(4 2)– 6(1 5)			275315.030	0.031	0.000	22.707	
19(2 17)– 18(3 16)		275361.911	275361.932	-0.021	5.442	117.022	a
26(4 22)– 25(5 21)		277176.960	277177.092	-0.132	4.170	221.534	a
17(1 16)– 16(2 15)		277381.139	277381.125	0.014	8.825	91.396	a
24(6 19)– 24(5 20)		280800.750	280800.982	-0.232	13.145	206.955	a
17(0 17)– 16(1 16)		281279.808	281279.792	0.016	14.417	86.083	a
23(6 18)– 23(5 19)		281561.594	281561.663	-0.069	12.459	192.873	a
21(6 15)– 21(5 16)		281809.784	281809.803	-0.019	11.121	166.488	b
27(1 26)– 27(0 27)		281862.636	281862.611	0.025	4.679	219.434	b
22(6 17)– 22(5 18)		282318.012	282317.994	0.018	11.781	179.383	a
9(3 7)– 8(2 6)		282613.879	282613.879	0.000	3.332	34.150	a
27(2 26)– 27(1 27)		282671.852	282671.821	0.031	4.678	219.462	b
20(6 14)– 20(5 15)		282947.166	282947.120	0.046	10.453	154.180	a
21(6 16)– 21(5 17)		283045.321	283045.257	0.064	11.110	166.485	a
17(1 17)– 16(0 16)		283188.143	283188.131	0.012	14.429	86.110	a
20(6 15)– 20(5 16)		283725.606	283725.531	0.075	10.447	154.179	a
19(6 13)– 19(5 14)		283870.266	283870.172	0.094	9.794	142.463	a
19(6 14)– 19(5 15)		284346.988	284346.943	0.045	9.790	142.463	a
18(6 12)– 18(5 13)		284619.642	284619.584	0.058	9.142	131.337	a
18(6 13)– 18(5 14)		284902.808	284902.752	0.056	9.140	131.337	a
17(6 11)– 17(5 12)		285227.832	285227.807	0.025	8.496	120.800	a
14(11 4)– 15(10 5)		285239.446	285239.418	0.028	0.341	166.697	a
14(11 3)– 15(10 6)		285239.446	285239.418	0.028	0.341	166.697	a
17(6 12)– 17(5 13)		285390.396	285390.391	0.005	8.495	120.800	a
15(2 14)– 14(1 13)		285650.535	285650.545	-0.010	7.272	72.960	a
16(6 10)– 16(5 11)		285720.653	285720.618	0.035	7.854	110.852	a
11(10 2)– 12(9 3)		285802.511	285802.474	0.037	0.128	125.651	a
11(10 1)– 12(9 4)		285802.511	285802.474	0.037	0.128	125.651	a
16(6 11)– 16(5 12)		285810.495	285810.520	-0.025	7.854	110.852	a
15(6 9)– 15(5 10)		286118.554	286118.508	0.046	7.215	101.492	a
15(6 10)– 15(5 11)		286166.139	286166.162	-0.023	7.215	101.492	a
14(6 9)– 14(5 10)		286462.079	286461.951	0.128	6.576	92.719	a
13(6 7)– 13(5 8)		286692.129	286692.013	0.116	5.935	84.534	a
13(6 8)– 13(5 9)		286703.307	286703.517	-0.210	5.935	84.534	a
12(6 6)– 12(5 7)		286891.976	286891.843	0.133	5.290	76.936	a
12(6 7)– 12(5 8)		286896.756	286896.995	-0.239	5.290	76.936	b
11(6 5)– 11(5 6)		287046.644	287046.525	0.119	4.635	69.923	a
11(6 6)– 11(5 7)		287048.460	287048.660	-0.200	4.635	69.923	b
10(6 4)– 10(5 5)		287163.970	287163.861	0.109	3.967	63.496	a
10(6 5)– 10(5 6)		287164.871	287164.667	0.204	3.967	63.496	a
9(6 3)– 9(5 4)		287250.703	287250.595	0.108	3.278	57.655	a
9(6 4)– 9(5 5)		287250.703	287250.865	-0.162	3.278	57.655	a
8(6 2)– 8(5 3)		287312.653	287312.611	0.042	2.558	52.399	a
8(6 3)– 8(5 4)		287312.653	287312.688	-0.035	2.558	52.399	a
7(6 1)– 7(5 2)		287355.099	287355.068	0.031	1.791	47.727	a
7(6 2)– 7(5 3)		287355.099	287355.086	0.013	1.791	47.727	a
6(6 0)– 6(5 1)		287382.475	287382.476	-0.001	0.953	43.641	a
6(6 1)– 6(5 2)		287382.475	287382.479	-0.004	0.953	43.641	a
3(3 1)– 2(0 2)			287847.185	0.027	0.000	11.350	
6(4 3)– 5(3 2)		287917.858	287918.069	-0.211	3.672	26.211	b
6(4 2)– 5(3 3)		287944.160	287944.599	-0.439	3.672	26.211	b
12(5 8)– 13(2 11)			290321.310	0.026	0.003	67.366	
9(3 6)– 8(2 7)			291738.151	0.013	3.159	34.178	
28(1 27)– 28(0 28)			293453.889	0.028	4.681	235.192	
28(2 27)– 28(1 28)			294039.348	0.028	4.680	235.212	
4(4 1)– 5(1 4)			295979.367	0.033	0.000	19.788	
23(3 20)– 22(4 19)			296715.581	0.028	4.665	172.132	
18(1 17)– 17(2 16)			297087.950	0.011	9.905	101.793	
10(3 8)– 9(2 7)			297167.074	0.014	3.494	40.002	
16(2 15)– 15(1 14)			297755.394	0.014	8.168	82.143	
18(0 18)– 17(1 17)			297796.617	0.011	15.438	96.043	
10(2 8)– 9(1 9)			298608.557	0.022	1.106	36.071	
18(1 18)– 17(0 17)			299161.069	0.011	15.446	96.062	
20(2 18)– 19(3 17)			300067.143	0.017	6.245	128.926	

TABLE 3. Observed and calculated transition frequencies for the ground vibrational state of *trans*-¹²CH₃¹²CH₂¹⁶OH — Continued

Transition		Freq. obs.	Freq. cal.	Uncertainty	Int.	Energy	Ref.
<i>J'</i>	<i>K_a' K_c'</i>	(MHz)	(MHz)	(MHz)	(<i>S</i>)	state (cm ⁻¹)	
19(6 14) – 20(3 17)			300473.775	0.035	0.011	142.463	
10(10 1) – 11(9 2)			303332.745	0.060	0.047	109.111	
10(10 0) – 11(9 3)			303332.745	0.060	0.047	109.111	
32(2 30) – 32(1 31)			303584.046	0.059	9.380	313.745	
29(1 28) – 29(0 29)			304997.252	0.030	4.683	251.489	
27(4 23) – 26(5 22)			305091.996	0.050	4.466	237.756	
7(4 4) – 6(3 3)			305353.741	0.013	3.808	30.301	
29(2 28) – 29(1 29)			305419.006	0.030	4.683	251.503	
7(4 3) – 6(3 4)			305433.631	0.013	3.808	30.301	
4(3 2) – 3(0 3)			305584.915	0.026	0.001	13.686	
17(2 16) – 16(1 15)		310246.976	310246.984	-0.008	9.124	91.883	a
11(3 9) – 10(2 8)		310904.665	310904.693	-0.028	3.669	46.441	a
10(3 7) – 9(2 8)		311289.915	311289.924	-0.009	3.199	40.053	a
11(5 7) – 12(2 10)			314155.428	0.025	0.002	60.348	
19(0 19) – 18(1 18)		314237.309	314237.305	0.004	16.455	106.544	a
19(1 19) – 18(0 18)		315207.238	315207.220	0.018	16.461	106.557	a
19(1 18) – 18(2 17)		316200.988	316201.006	-0.018	10.996	112.724	a
30(1 29) – 30(0 30)		316502.183	316502.115	0.068	4.686	268.326	b
30(2 29) – 30(1 30)		316804.823	316804.755	0.068	4.685	268.336	b
5(5 1) – 4(4 0)		322690.784	322690.785	-0.001	4.487	30.551	a
5(5 0) – 4(4 1)		322690.784	322690.802	-0.018	4.487	30.551	a
8(4 5) – 7(3 4)		322721.463	322721.524	-0.061	3.953	34.977	a
8(4 4) – 7(3 5)		322921.844	322921.842	0.002	3.951	34.977	a
18(2 17) – 17(1 16)		323194.444	323194.448	-0.004	10.123	102.177	a
5(3 3) – 4(0 4)			323627.711	0.025	0.004	16.607	
12(3 10) – 11(2 9)		323821.309	323821.351	-0.042	3.864	53.466	a
21(2 19) – 20(3 18)		324318.960	324319.035	-0.075	7.137	141.385	a
24(3 21) – 23(4 20)		324318.960	324319.068	-0.108	5.213	186.550	a
18(6 13) – 19(3 16)			327263.882	0.034	0.008	131.337	
31(1 30) – 31(0 31)		327975.785	327975.717	0.068	4.688	285.702	b
31(2 30) – 31(1 31)		328192.173	328192.115	0.058	4.687	285.710	b
11(2 9) – 10(1 10)		328887.139	328887.110	0.029	0.946	42.664	a
20(0 20) – 19(1 19)		330621.119	330621.095	0.024	17.470	117.586	a
20(1 20) – 19(0 19)		331307.079	331307.054	0.025	17.473	117.595	a
11(3 8) – 10(2 9)		331655.238	331655.225	0.013	3.191	46.529	a
28(4 24) – 27(5 23)		333755.208	333755.030	0.178	4.808	254.593	a
20(1 19) – 19(2 18)		334769.040	334769.056	-0.016	12.086	124.188	a
13(3 11) – 12(2 10)		335949.642	335949.708	-0.066	4.088	61.075	a
19(2 18) – 18(1 17)		336626.380	336626.378	0.002	11.151	113.022	a
21(7 14) – 21(6 15)		336767.404	336767.115	0.289	10.566	177.721	a
20(7 13) – 20(6 14)		337286.523	337286.324	0.199	9.921	165.431	a
20(7 14) – 20(6 15)		337323.095	337323.405	-0.310	9.921	165.431	a
10(5 6) – 11(2 9)			337366.647	0.025	0.001	53.918	
19(7 12) – 19(6 13)		337727.095	337726.936	0.159	9.279	153.729	a
19(7 13) – 19(6 14)		337747.000	337747.148	-0.148	9.279	153.729	a
18(7 11) – 18(6 12)		338099.257	338099.109	0.148	8.640	142.615	a
18(7 12) – 18(6 13)		338109.673	338109.734	-0.061	8.640	142.615	a
17(7 10) – 17(6 11)			338411.510	0.017	8.001	132.088	
17(7 11) – 17(6 12)			338416.875	0.017	8.001	132.088	
16(7 9) – 16(6 10)		338671.752	338671.665	0.087	7.362	122.149	a
16(7 10) – 16(6 11)		338674.228	338674.252	-0.024	7.362	122.149	a
15(7 8) – 15(6 9)		338886.208	338886.205	0.003	6.719	112.796	a
14(7 7) – 14(6 8)		339061.261	339061.056	0.205	6.071	104.029	a
14(7 8) – 14(6 9)		339061.261	339061.567	-0.306	6.071	104.029	a
13(7 6) – 13(6 7)		339201.642	339201.558	0.084	5.415	95.849	a
13(7 7) – 13(6 8)		339201.642	339201.764	-0.122	5.415	95.849	a
12(7 5) – 12(6 6)		339312.570	339312.563	0.007	4.747	88.254	a
12(7 6) – 12(6 7)		339312.570	339312.639	-0.069	4.747	88.254	a
11(7 4) – 11(6 5)		339398.451	339398.485	-0.034	4.062	81.244	a
11(7 5) – 11(6 6)		339398.451	339398.510	-0.059	4.062	81.244	a
32(1 31) – 32(0 32)		339423.434	339423.577	-0.143	4.690	303.618	a
10(7 3) – 10(6 4)		339463.309	339463.345	-0.036	3.352	74.820	a
10(7 4) – 10(6 5)		339463.309	339463.353	-0.044	3.352	74.820	a
9(7 2) – 9(6 3)		339510.737	339510.799	-0.062	2.610	68.980	a

TABLE 3. Observed and calculated transition frequencies for the ground vibrational state of *trans*-¹²CH₃¹²CH₂¹⁶OH — Continued

Transition		Freq. obs.	Freq. cal.	Uncertainty	Int.	Energy	Ref.
<i>J'</i>	<i>K_a' K_c'</i>	(MHz)	(MHz)	(MHz)	(<i>S</i>)	'state (cm ⁻¹)	
9(7 3)– 9(6 4)		339510.737	339510.800	–0.063	2.610	68.980	a
8(7 1)– 8(6 2)		339544.095	339544.147	–0.052	1.820	63.725	a
8(7 2)– 8(6 3)		339544.095	339544.147	–0.052	1.820	63.725	a
7(7 0)– 7(6 1)		339566.321	339566.352	–0.031	0.961	59.054	a
7(7 1)– 7(6 2)		339566.321	339566.352	–0.031	0.961	59.054	a
32(2 31)– 32(1 32)		339577.859	339577.809	0.050	4.690	303.624	a
9(4 6)– 8(3 5)		339978.879	339978.937	–0.058	4.101	40.239	a
6(5 2)– 5(4 1)		340189.261	340189.225	0.036	4.543	34.054	a
6(5 1)– 5(4 2)		340189.261	340189.378	–0.117	4.543	34.054	a
9(4 5)– 8(3 6)		340420.368	340420.389	–0.021	4.097	40.240	a
6(3 4)– 5(0 5)			342152.851	0.023	0.010	20.113	
21(0 21)– 20(1 20)		346962.594	346962.578	0.016	18.482	129.169	a
14(3 12)– 13(2 11)		347350.929	347351.139	–0.210	4.349	69.268	a
21(1 21)– 20(0 20)		347445.523	347445.541	–0.018	18.484	129.175	a
22(2 20)– 21(3 19)		347974.642	347974.697	–0.055	8.109	154.391	a
20(2 19)– 19(1 18)			350534.319	0.014	12.195	124.416	
33(1 32)– 33(0 33)			350849.875	0.074	4.692	322.074	
25(3 22)– 24(4 21)			351917.591	0.036	5.843	201.548	
21(1 20)– 20(2 19)			352858.203	0.014	13.169	136.186	
12(3 9)– 11(2 10)			353034.503	0.015	3.128	53.609	
17(6 12)– 18(3 15)			353283.343	0.032	0.006	120.800	
10(4 7)– 9(3 6)			357067.453	0.014	4.246	46.088	
7(5 3)– 6(4 2)			357681.199	0.014	4.642	38.142	
7(5 2)– 6(4 3)			357681.966	0.014	4.642	38.142	
10(4 6)– 9(3 7)			357950.252	0.014	4.237	46.090	
15(3 13)– 14(2 12)			358107.432	0.019	4.657	78.043	
9(5 5)– 10(2 8)			359837.390	0.025	0.001	48.073	
12(2 10)– 11(1 11)			360998.908	0.027	0.800	49.869	
7(3 5)– 6(0 6)			361361.710	0.022	0.021	24.205	
22(0 22)– 21(1 21)			363272.643	0.017	19.492	141.293	
22(1 22)– 21(0 21)			363611.332	0.017	19.494	141.297	
21(2 20)– 20(1 19)			364881.851	0.016	13.245	136.359	
16(3 14)– 15(2 13)			368315.578	0.019	5.020	87.397	
22(1 21)– 21(2 20)			370541.190	0.016	14.243	148.719	
23(2 21)– 22(3 20)			370919.822	0.020	9.147	167.937	
11(4 8)– 10(3 7)			373909.915	0.014	4.386	52.526	
8(5 4)– 7(4 3)			375161.391	0.014	4.765	42.815	
8(5 3)– 7(4 4)			375164.211	0.014	4.765	42.815	
11(4 7)– 10(3 8)			375545.141	0.014	4.369	52.529	
13(3 10)– 12(2 11)			375641.541	0.017	3.009	61.299	
17(3 15)– 16(2 14)			378085.709	0.020	5.445	97.330	
16(6 11)– 17(3 14)			378394.226	0.030	0.004	110.852	
26(3 23)– 25(4 22)			379327.966	0.041	6.562	217.118	
23(0 23)– 22(1 22)			379559.299	0.020	20.501	153.958	
22(2 21)– 21(1 20)			379615.695	0.018	14.295	148.849	
23(1 23)– 22(0 22)			379795.970	0.020	20.502	153.961	
8(3 6)– 7(0 7)			381461.476	0.021	0.037	28.884	
18(3 16)– 17(2 15)			387541.009	0.021	5.942	107.837	
23(1 22)– 22(2 21)			387889.425	0.018	15.306	161.788	
12(4 9)– 11(3 8)			390409.409	0.015	4.520	59.552	
17(8 9)– 17(7 10)			391033.170	0.025	7.502	145.132	
17(8 10)– 17(7 11)			391033.286	0.025	7.502	145.132	
16(8 8)– 16(7 9)			391192.013	0.023	6.852	135.198	
16(8 9)– 16(7 10)			391192.062	0.023	6.852	135.198	
15(8 7)– 15(7 8)			391322.782	0.022	6.195	125.849	
15(8 8)– 15(7 9)			391322.801	0.022	6.195	125.849	
14(8 6)– 14(7 7)			391428.944	0.021	5.527	117.086	
14(8 7)– 14(7 8)			391428.951	0.021	5.527	117.086	
13(8 5)– 13(7 6)			391513.719	0.019	4.844	108.908	
13(8 6)– 13(7 7)			391513.721	0.019	4.844	108.908	
12(8 4)– 12(7 5)			391580.092	0.018	4.142	101.315	
12(8 5)– 12(7 6)			391580.092	0.018	4.142	101.315	
11(8 3)– 11(7 4)			391630.821	0.017	3.415	94.308	
11(8 4)– 11(7 5)			391630.821	0.017	3.415	94.308	

TABLE 3. Observed and calculated transition frequencies for the ground vibrational state of *trans*-¹²CH₃¹²CH₂¹⁶OH — Continued

Transition		Freq. obs.	Freq. cal.	Uncertainty	Int.	Energy	Ref.
<i>J'</i>	<i>K_a' K_c'</i>	(MHz)	(MHz)	(MHz)	(<i>S</i>)	'state (cm ⁻¹)	
10(8 2)– 10(7 3)			391668.443	0.018	2.652	87.884	
10(8 3)– 10(7 4)			391668.443	0.018	2.652	87.884	
9(8 1)– 9(7 2)			391695.279	0.020	1.843	82.045	
9(8 2)– 9(7 3)			391695.279	0.020	1.843	82.045	
8(8 0)– 8(7 1)			391713.434	0.024	0.968	76.791	
8(8 1)– 8(7 2)			391713.434	0.024	0.968	76.791	
6(6 1)– 5(5 0)			392404.976	0.019	5.487	43.641	
6(6 0)– 5(5 1)			392404.977	0.019	5.487	43.641	
9(5 5)– 8(4 4)			392622.767	0.015	4.903	48.073	
9(5 4)– 8(4 5)			392631.250	0.015	4.903	48.073	
24(2 22)– 23(3 21)			393079.704	0.023	10.236	182.019	
12(4 8)– 11(3 9)			393254.404	0.015	4.488	59.559	
23(2 22)– 22(1 21)			394675.800	0.020	15.343	161.884	
13(2 11)– 12(1 12)			394886.358	0.030	0.673	57.682	
24(0 24)– 23(1 23)			395828.366	0.023	21.509	167.165	
24(1 24)– 23(0 23)			395993.223	0.023	21.510	167.167	
19(3 17)– 18(2 16)			396817.916	0.021	6.517	118.917	
14(3 11)– 13(2 12)			399690.238	0.019	2.836	69.602	
16(3 13)– 15(6 10)			402506.608	0.028	0.003	101.492	
9(3 7)– 8(0 8)			402642.906	0.020	0.058	34.150	
24(1 23)– 23(2 22)			404968.039	0.022	16.361	175.393	
20(3 18)– 19(2 17)			406064.854	0.022	7.176	130.567	
27(3 24)– 26(4 23)			406365.907	0.047	7.374	233.251	
13(4 10)– 12(3 9)			406450.925	0.015	4.645	67.167	
7(6 2)– 6(5 1)			409904.952	0.018	5.532	47.727	
7(6 1)– 6(5 2)			409904.956	0.018	5.532	47.727	
24(2 23)– 23(1 22)			410002.793	0.023	16.386	175.464	
10(5 6)– 9(4 5)			410056.049	0.015	5.047	53.918	
10(5 5)– 9(4 6)			410078.144	0.015	5.047	53.918	
13(4 9)– 12(3 10)			411145.839	0.015	4.590	67.180	
25(0 25)– 24(1 24)			412084.026	0.027	22.516	180.913	
25(1 25)– 24(0 24)			412198.531	0.027	22.516	180.914	
25(2 23)– 24(3 22)			414424.832	0.026	11.356	196.631	
21(3 19)– 20(2 18)			415437.933	0.023	7.921	142.784	
22(7 16)– 23(4 19)			419443.464	0.052	0.009	190.600	
25(1 24)– 24(2 23)			421833.470	0.026	17.406	189.535	
14(4 11)– 13(3 10)			421907.136	0.016	4.763	75.372	
10(3 8)– 9(0 9)			425059.494	0.020	0.084	40.002	
22(3 20)– 21(2 19)			425092.742	0.025	8.750	155.565	
15(3 12)– 14(2 13)			425377.295	0.020	2.618	78.523	
25(2 24)– 24(1 23)			425542.545	0.027	17.424	189.587	
14(6 9)– 15(3 12)			425585.616	0.025	0.002	92.719	
8(6 3)– 7(5 2)			427400.803	0.018	5.618	52.399	
8(6 2)– 7(5 3)			427400.821	0.018	5.618	52.399	
11(5 7)– 10(4 6)			427448.908	0.015	5.194	60.348	
11(5 6)– 10(4 7)			427500.522	0.015	5.194	60.348	
26(0 26)– 25(1 25)			428329.248	0.032	23.522	195.202	
26(1 26)– 25(0 25)			428408.574	0.032	23.522	195.203	
14(4 10)– 13(3 11)			429308.332	0.016	4.668	75.395	
14(2 12)– 13(1 13)			430456.521	0.031	0.368	66.098	
28(3 25)– 27(4 24)			432853.405	0.054	8.278	249.938	
26(2 24)– 25(3 23)			434969.408	0.030	12.490	211.773	
23(3 21)– 22(2 20)			435172.638	0.027	9.656	168.907	
15(4 12)– 14(3 11)			436648.987	0.017	4.874	84.167	
26(1 25)– 25(2 24)			438532.815	0.031	18.445	204.215	
26(2 25)– 25(1 24)			441248.348	0.032	18.457	204.253	
11(9 2)– 11(8 3)			443782.064	0.023	2.688	109.111	
11(9 3)– 11(8 4)			443782.064	0.023	2.688	109.111	
10(9 1)– 10(8 2)			443803.766	0.027	1.862	102.688	
10(9 2)– 10(8 3)			443803.766	0.027	1.862	102.688	
9(9 0)– 9(8 1)			443818.479	0.032	0.974	96.850	
9(9 1)– 9(8 2)			443818.479	0.032	0.974	96.850	
27(0 27)– 26(1 26)			444566.115	0.037	24.528	210.032	
27(1 27)– 26(0 26)			444620.941	0.037	24.528	210.033	

TABLE 3. Observed and calculated transition frequencies for the ground vibrational state of *trans*-¹²CH₃¹²CH₂¹⁶OH — Continued

Transition		Freq. obs.	Freq. cal.	Uncertainty	Int.	Energy	Ref.
<i>J'</i>	<i>K'_a' K'_c' J''</i>	(MHz)	(MHz)	(MHz)	(<i>S</i>)	'state (cm ⁻¹)	
21(7 15)– 22(444637.123	0.043	0.006	177.721	
12(5 8)– 11(444784.845	0.016	5.341	67.366	
9(6 4)– 8(444889.615	0.018	5.730	57.655	
9(6 3)– 8(444889.694	0.018	5.730	57.655	
12(5 7)– 11(444895.470	0.016	5.340	67.366	
24(3 22)– 23(445795.578	0.029	10.628	182.807	
13(6 8)– 14(447652.799	0.023	0.001	84.534	
15(4 11)– 14(447854.139	0.017	4.716	84.207	
11(3 9)– 10(448814.181	0.021	0.111	46.441	
16(4 13)– 15(450560.182	0.019	4.984	93.553	
16(3 13)– 15(452863.898	0.022	2.371	88.066	
27(2 25)– 26(454763.596	0.035	13.627	227.443	
27(1 26)– 26(455104.273	0.036	19.478	219.434	
25(3 23)– 24(457042.868	0.033	11.650	197.264	
27(2 26)– 26(457081.449	0.037	19.487	219.462	
4(4 1)– 3(458532.118	0.034	0.000	19.788	
28(0 28)– 27(460796.070	0.043	25.532	225.403	
28(1 28)– 27(460833.882	0.043	25.533	225.404	
13(5 9)– 12(462041.677	0.016	5.485	74.971	
7(7 0)– 6(462088.829	0.024	6.487	59.054	
7(7 1)– 6(462088.829	0.024	6.487	59.054	
13(5 8)– 12(462262.711	0.016	5.484	74.971	
10(6 5)– 9(462367.878	0.017	5.858	63.496	
10(6 4)– 9(462368.157	0.017	5.858	63.496	
17(4 14)– 16(463552.605	0.020	5.097	103.528	
4(4 0)– 3(465823.207	0.034	0.000	19.788	
16(4 12)– 15(466920.570	0.018	4.729	93.618	
15(2 13)– 14(467586.791	0.032	0.481	75.112	
20(7 14)– 21(468677.723	0.038	0.005	165.431	
12(6 7)– 13(468779.712	0.022	0.001	76.936	
26(3 24)– 25(468953.177	0.037	12.707	212.274	
28(1 27)– 27(471578.138	0.043	20.507	235.192	
28(2 27)– 27(473010.619	0.043	20.512	235.212	
5(4 2)– 4(473771.467	0.032	0.000	22.707	
28(2 26)– 27(473882.200	0.041	14.756	243.642	
12(3 10)– 11(473956.711	0.022	0.138	53.466	
18(4 15)– 17(475578.472	0.022	5.222	114.094	
29(0 29)– 28(477020.095	0.051	26.537	241.315	
29(1 29)– 28(477046.122	0.051	26.537	241.316	
14(5 10)– 13(479189.610	0.017	5.625	83.164	
8(7 1)– 7(479589.883	0.023	6.524	63.725	
8(7 2)– 7(479589.883	0.023	6.524	63.725	
14(5 9)– 13(479606.096	0.017	5.622	83.165	
11(6 6)– 10(479831.436	0.018	5.996	69.923	
11(6 5)– 10(479832.274	0.018	5.996	69.923	
27(3 25)– 26(481523.521	0.041	13.783	227.835	
17(3 14)– 16(482260.818	0.024	2.110	98.230	
5(4 1)– 4(485917.932	0.032	0.000	22.707	
19(4 16)– 18(486635.789	0.023	5.369	125.248	
17(4 13)– 16(486670.577	0.019	4.700	103.631	
29(1 28)– 28(487977.999	0.050	21.531	251.489	
6(4 3)– 5(488560.589	0.030	0.001	26.211	
29(2 28)– 28(489011.238	0.051	21.535	251.503	
19(7 13)– 20(491636.082	0.036	0.004	153.729	
29(2 27)– 28(492412.881	0.049	15.875	260.370	
30(0 30)– 29(493238.842	0.059	27.541	257.768	
30(1 30)– 29(493256.725	0.059	27.541	257.769	
28(3 26)– 27(494716.423	0.047	14.869	243.945	
10(10 0)– 10(495876.159	0.055	0.978	119.229	
10(10 1)– 10(495876.159	0.055	0.978	119.229	
15(5 11)– 14(496188.930	0.018	5.758	91.946	
20(4 17)– 19(496766.403	0.026	5.547	136.991	
15(5 10)– 14(496935.411	0.018	5.752	91.948	
9(7 3)– 8(497087.804	0.021	6.599	68.980	

TABLE 3. Observed and calculated transition frequencies for the ground vibrational state of *trans*-¹²CH₃¹²CH₂¹⁶OH — Continued

Transition		Freq. obs. (MHz)	Freq. cal. (MHz)	Uncertainty (MHz)	Int. (S)	Energy state (cm ⁻¹)	Ref.
J'	K _a ' K _c ' J''						
9(7 2) - 8(497087.805	0.021	6.599	68.980	
12(6 7) - 11(497275.403	0.018	6.141	76.936	
12(6 6) - 11(497277.641	0.018	6.141	76.936	
13(3 11) - 12(500490.036	0.024	0.161	61.075	
7(4 4) - 6(502978.274	0.029	0.002	30.301	
30(1 29) - 29(504321.951	0.059	22.552	268.326	
21(4 18) - 20(506048.815	0.028	5.767	149.320	
16(2 14) - 15(506128.092	0.033	0.412	84.718	
6(4 2) - 5(506763.669	0.031	0.001	26.211	
18(4 14) - 17(507291.511	0.021	4.621	114.251	
31(0 31) - 30(509452.731	0.070	28.544	274.762	
16(5 12) - 15(512987.422	0.018	5.883	101.318	
18(7 12) - 19(513617.604	0.035	0.003	142.615	
18(3 15) - 17(513620.524	0.026	1.853	109.016	
16(5 11) - 15(514268.482	0.018	5.873	101.321	
10(7 4) - 9(514580.636	0.021	6.701	74.820	
10(7 3) - 9(514580.638	0.021	6.701	74.820	
22(4 19) - 21(514589.277	0.031	6.039	162.234	
13(6 8) - 12(514694.032	0.018	6.288	84.534	
13(6 7) - 12(514699.469	0.018	6.288	84.534	
8(4 5) - 7(517123.248	0.027	0.004	34.977	
23(4 20) - 22(522514.098	0.035	6.371	175.732	
32(0 32) - 31(525662.017	0.082	29.548	292.297	
14(3 12) - 13(528381.227	0.025	0.180	69.268	
7(4 3) - 6(528421.472	0.029	0.001	30.301	
19(4 15) - 18(528991.059	0.022	4.487	125.482	
17(5 13) - 16(529517.834	0.019	6.000	111.280	
24(4 21) - 23(529964.513	0.039	6.772	189.809	
9(4 6) - 8(531116.387	0.025	0.007	40.239	
17(5 12) - 16(531633.529	0.019	5.982	111.286	
8(8 0) - 7(531736.964	0.027	7.487	76.791	
8(8 1) - 7(531736.964	0.027	7.487	76.791	
11(7 5) - 10(532066.084	0.021	6.820	81.244	
11(7 4) - 10(532066.092	0.021	6.820	81.244	
14(6 9) - 13(532080.491	0.019	6.435	92.719	
14(6 8) - 13(532092.722	0.019	6.435	92.719	
17(7 11) - 18(534746.458	0.034	0.002	132.088	
25(4 22) - 24(537093.902	0.045	7.251	204.465	
26(4 23) - 25(544066.189	0.051	7.813	219.696	
10(4 7) - 9(545102.708	0.024	0.013	46.088	
18(5 14) - 17(545695.881	0.020	6.107	121.833	
17(2 15) - 16(545906.607	0.033	0.357	94.910	
19(3 16) - 18(546937.218	0.028	1.613	120.420	
18(5 13) - 17(549071.717	0.020	6.076	121.843	
9(8 1) - 8(549238.936	0.025	7.517	82.045	
9(8 2) - 8(549238.936	0.025	7.517	82.045	
15(6 10) - 14(549426.546	0.020	6.582	101.492	
15(6 9) - 14(549452.342	0.020	6.582	101.492	
12(7 6) - 11(549541.517	0.021	6.951	88.254	
12(7 5) - 11(549541.544	0.021	6.951	88.254	
8(4 4) - 7(550960.082	0.028	0.002	34.977	
20(4 16) - 19(551989.357	0.024	4.298	137.330	
16(7 10) - 17(555151.256	0.032	0.001	122.149	
15(3 13) - 14(557572.571	0.027	0.194	78.043	
11(4 8) - 10(559252.498	0.024	0.022	52.526	
19(5 15) - 18(561419.623	0.021	6.203	132.978	
19(5 14) - 18(566639.806	0.021	6.153	132.995	
16(6 11) - 15(566722.081	0.020	6.726	110.852	
10(8 2) - 9(566738.281	0.025	7.584	87.884	
10(8 3) - 9(566738.281	0.025	7.584	87.884	
16(6 10) - 15(566773.577	0.020	6.725	110.852	
13(7 7) - 12(567003.953	0.022	7.090	95.849	
13(7 6) - 12(567004.032	0.022	7.090	95.849	
12(4 9) - 11(573760.599	0.024	0.035	59.552	

TABLE 3. Observed and calculated transition frequencies for the ground vibrational state of *trans*-¹²CH₃¹²CH₂¹⁶OH — Continued

Transition			Freq. obs.	Freq. cal.	Uncertainty	Int.	Energy	Ref.
<i>J'</i>	<i>K_a'</i>	<i>K_c'</i>	(MHz)	(MHz)	(MHz)	(<i>S</i>)	'state (cm ⁻¹)	
<i>J''</i>	<i>K_a''</i>	<i>K_c''</i>						
9(4 5) – 8(1 8)				574454.381	0.027	0.003	40.240	
15(7 9) – 16(4 12)				574954.382	0.030	0.001	112.796	
21(4 17) – 20(3 18)				576506.756	0.027	4.055	149.797	
20(5 16) – 19(4 15)				576571.269	0.023	6.289	144.715	
20(3 17) – 19(2 18)				582152.747	0.030	1.397	132.440	
17(6 12) – 16(5 11)				583954.437	0.021	6.865	120.800	
17(6 11) – 16(5 12)				584052.459	0.021	6.865	120.800	
11(8 3) – 10(7 4)				584233.560	0.025	7.676	94.308	
11(8 4) – 10(7 3)				584233.560	0.025	7.676	94.308	
20(5 15) – 19(4 16)				584412.804	0.023	6.209	144.742	
14(7 8) – 13(6 7)				584450.045	0.023	7.234	104.029	
14(7 7) – 13(6 8)				584450.260	0.023	7.234	104.029	
18(2 16) – 17(1 17)				586725.563	0.032	0.314	105.681	
16(3 14) – 15(0 15)				587990.498	0.028	0.204	87.397	
13(4 10) – 12(1 11)				588842.562	0.025	0.055	67.167	
21(5 17) – 20(4 16)				591022.485	0.025	6.366	157.044	
14(7 8) – 15(4 11)				594265.546	0.028	0.001	104.029	
10(4 6) – 9(1 9)				598984.110	0.027	0.005	46.090	

Notes: References a) and b) refer to the present work. Reference b) indicates that an average of a measured torsional doublet has been taken. The listed state energy in cm⁻¹ is for the upper state. The uncertainties are calculated for those transitions that have not been measured. For those transitions that have been measured, residuals (observed – calculated frequencies) appear in the uncertainty column.

TABLE 4. Rotational and centrifugal distortion constants for the ground vibrational state of *trans*-ethanol

Constant	This work	Uncert.	Lovas ref. [27]	Uncert.
	(MHz)	(1σ)	(MHz)	(1σ)
<i>A</i>	34891.7707	(40)	34891.7542	(197)
<i>B</i>	9350.6776	(6)	9350.6752	(61)
<i>C</i>	8135.2352	(3)	8135.2313	(58)
Δ_J	0.00853736	(76)	0.0085523	(749)
Δ_{JK}	-0.0287785	(300)	-0.028410	(677)
Δ_K	0.252460	(120)	0.251542	(488)
δ_J	0.00173766	(46)	0.0017397	(106)
δ_K	0.0066814	(240)	0.008246	(1007)
$H_J \times 10^6$			0.1231	(2403)
$H_{JK} \times 10^6$	1.050	(44)	15.10	(719)
$H_{KJ} \times 10^6$	-13.73	(83)	-50.59	(1276)
$H_K \times 10^6$	33.20	(87)	58.52	(1240)
$h_J \times 10^6$	-0.00475	(36)	0.5682	(3577)
$h_{JK} \times 10^6$	0.305	(29)	-4.539	(5190)
$h_K \times 10^6$	61.75	(74)	326.3	(1133)
$L_{JK} \times 10^9$	-6.67	(89)		
$L_{KKJ} \times 10^9$	-36.8	(49)		

Notes: The analysis of Lovas [27] has been redone by the referee to include new low frequency data and similar fourth-order distortion constants to those utilized here. The uncertainties are written without decimal points and refer to the right-most significant figures of the respective constants.

TABLE 5. Maximum J values for the unperturbed energy levels of the ground vibrational state of *trans*-ethanol

K_a Quantum number	Maximum J
0	33
1	32
2	30
3	29
4	28
5	26
6	24
7	21
8	18
9	15
10	11
11	None

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