# 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 *v*=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 sub-millimeter-wave region [30]. Therefore, a systematic study of the rotational spectrum in the millimeter-wave and submil-limeter-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 ($V_3 \approx 1164$ 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 ± 5.0 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 ($\mu_a \approx 0.046$ *D*), we and earlier
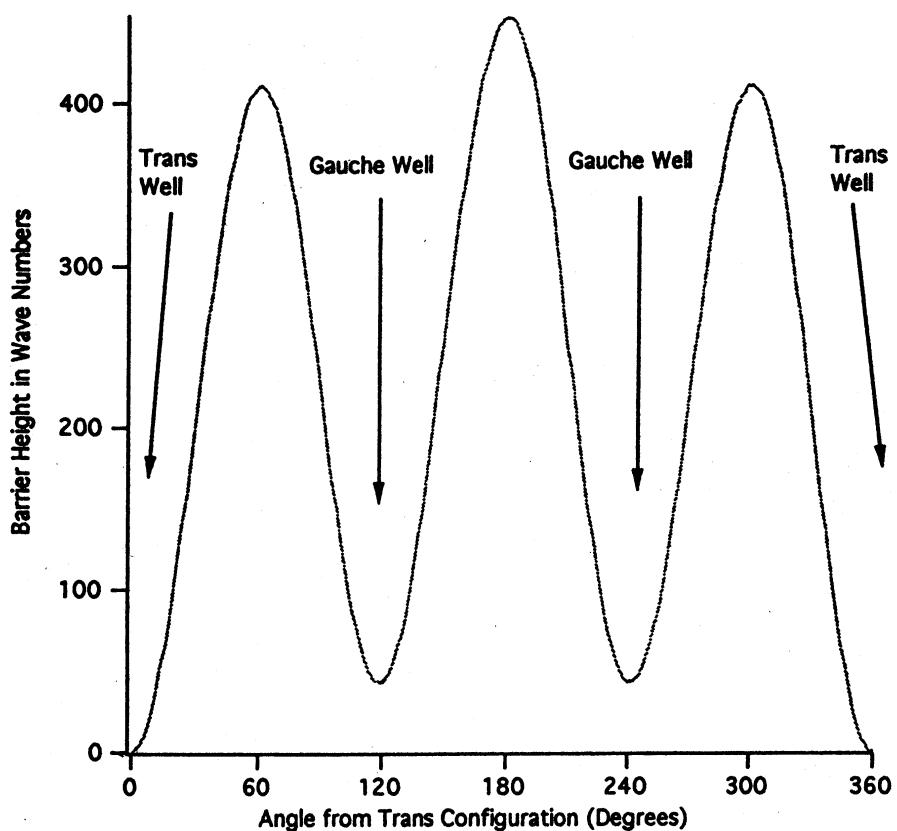
FIG. 1. Hydroxyl barrier. The potential energy for internal rotation of the hydroxyl group in ethyl alcohol is shown as a function of torsional angle. The two different *gauche* wells are of equal depth and lie above the *trans* well [26].
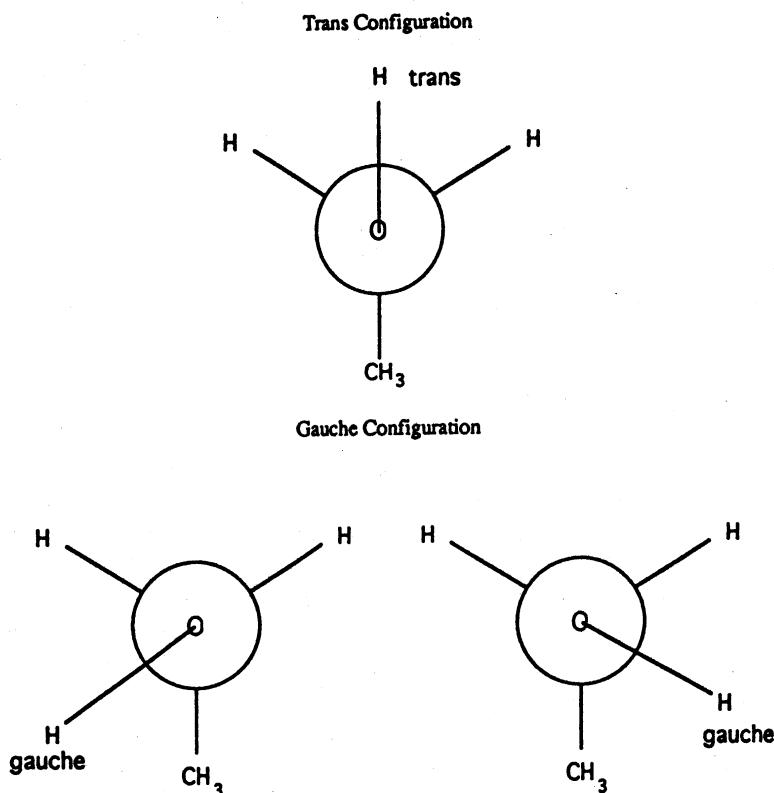


FIG. 2. Hydroxyl position. The position of the hydroxyl group looking down the CO bond in ethyl alcohol is shown for the *trans* and *gauche* configurations. The *gauche+* state is characterized by the symmetric superposition of wave functions peaking at the *gauche* hydrogen positions while the *gauche−*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

Gauche-

~1 MHz

3.2 cm$^{-1}$

Gauche+

~1 MHz

Asymmetric
Rotor Level
J, K$_a$, K$_c$

41.2 cm$^{-1}$

Trans

~1 MHz

Effect of
OH Torsion

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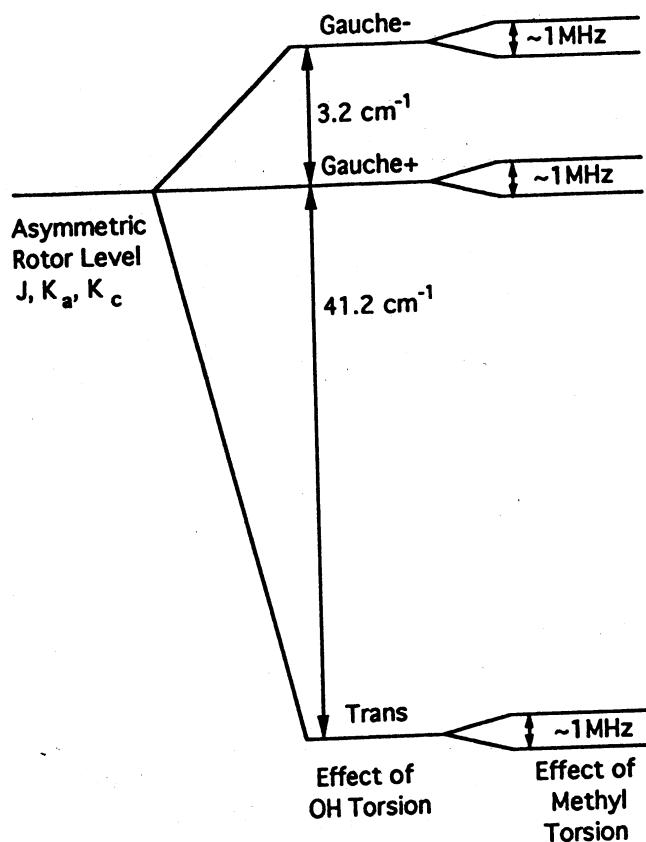
FIG. 3. Ground state rotational-torsional energy levels. The splittings of asymmetric rotor levels in the ground vibrational state of ethanol due to the effects of OH and methyl torsional motions are depicted. The splittings due to the methyl torsional motion are representative values.

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 $|K_a> \pm |-K_a>$ (neglecting the mixing of other $K_a$ values), and torsional-rotational interaction, leading to wave functions characterized by $|K_a>$ and $|-K_a>$. 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.
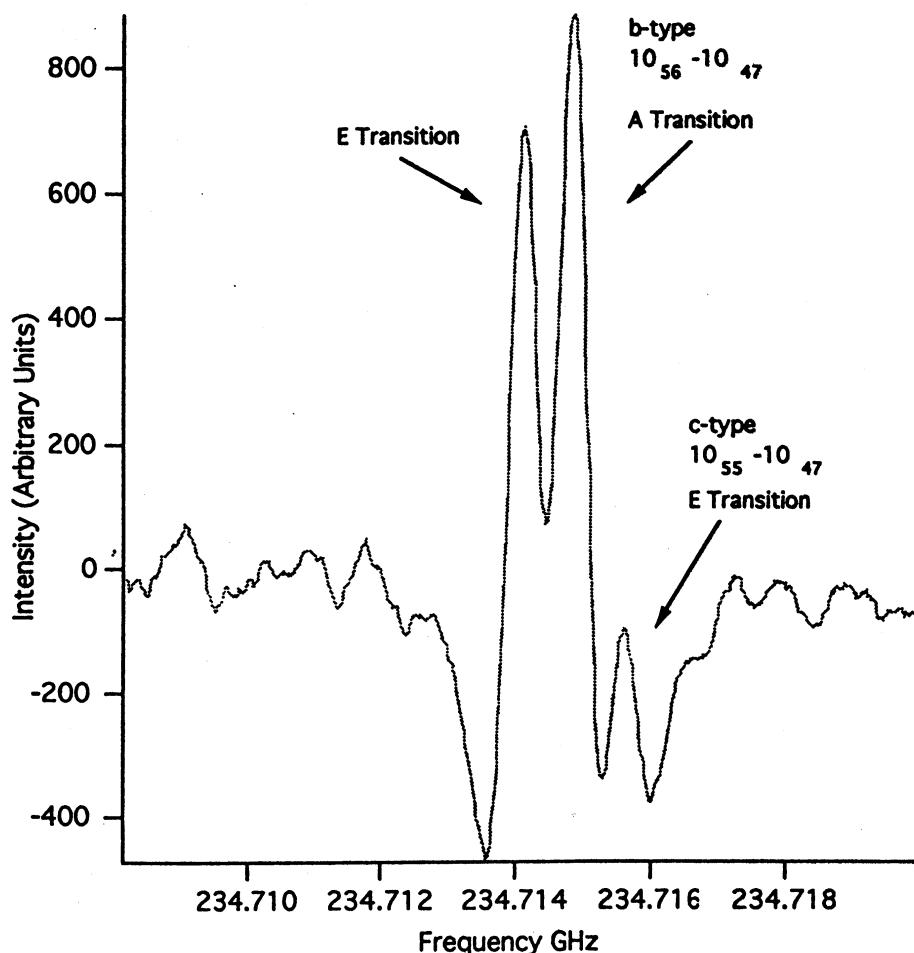


FIG. 4. Triplet spectrum. A completely resolved $Q$-branch spectral triplet at 234.7 GHz is shown. The splitting of the b-type transitions in the $A$ and $E$ torsional substates as well as the appearance of a c-type spectral transition is caused by the effects of methyl internal rotation.

## 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 $\rho$ 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 $\rho$, 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 CH$_3$ 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, vitually all of the measured $b$-type trans lines were fit with a Watson $A$-reduced Hamiltonian in the $I^r$ 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.

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 |
| E | 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 |

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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 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 | 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 | 111287.023 | 111287.096 | −0.073 |
| E | 17 | 3 | 15 | 16 | 4 | 12 | 111287.303 | 111287.376 | −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 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 | 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 |
| A | 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 |
| A | 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 |
| E | 11 | 6 | 6  | 11 | 5 | 7  | 287048.861 | 287048.768 | 0.093 |
| A | 11 | 6 | 6  | 11 | 5 | 7  | 287048.861 | 287049.020 | −0.159 |
| E | 11 | 6 | 5  | 11 | 5 | 7  | 287917.406 | 287917.501 | −0.095 |
| E | 6  | 4 | 3  | 5  | 3 | 2  | 287918.309 | 287918.352 | −0.043 |
| A | 6  | 4 | 3  | 5  | 3 | 2  | 287919.212 | 287919.043 | 0.169 |
| E | 6  | 4 | 2  | 5  | 3 | 2  | 287943.287 | 287943.312 | −0.025 |
| E | 6  | 4 | 3  | 5  | 3 | 3  | 287944.832 | 287944.882 | −0.050 |
| A | 6  | 4 | 2  | 5  | 3 | 3  | 287944.832 | 287944.853 | −0.021 |
| E | 6  | 4 | 2  | 5  | 3 | 3  | 316501.850 | 316501.898 | −0.048 |
| E | 30 | 1 | 29 | 30 | 0 | 30 | 316502.515 | 316502.535 | −0.020 |
| A | 30 | 1 | 29 | 30 | 0 | 30 | 316804.487 | 316804.498 | −0.011 |
| E | 30 | 2 | 29 | 30 | 1 | 30 | 316805.158 | 316805.133 | 0.025 |
| A | 30 | 2 | 29 | 30 | 1 | 30 |  |  |  |

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$\sigma$) | Units |
|---|---|---|---|
| $A$ | 34106.87786 | (96000) | |
| $B$ | 10137.36448 | (96000) | |
| $C$ | 8133.409785 | (1200) | |
| $D_{ab}$ | 4409.960070 | (2600000) | |
| $F$ | 6.47394 | (Fixed) | cm$^{-1}$ |
| $\rho$ | 0.18687 | (210) | unitless |
| $V_3$ | 1173.76 | (220) | cm$^{-1}$ |
| $\Delta_{JK}$ | −0.06455670 | (4600) | |
| $\Delta_J$ | 0.009453058 | (2700) | |
| $\Delta_K$ | 0.30251487 | (11000) | |
| $\delta_J$ | 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 $trans$-$^{12}CH_3{}^{12}CH_2{}^{16}OH$

| 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-$^{12}CH_3{}^{12}CH_2{}^{16}OH$ — Continued

| Transition J' $K_a'$ $K_c'$ — J" $K_a"$ $K_c"$ | Freq. obs. (MHz) | Freq. cal. (MHz) | Uncertainty (MHz) | Int. (S) | Energy 'state (cm$^{-1}$) | Ref. |
|---|---|---|---|---|---|---|
| 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 $trans$-$^{12}CH_3{}^{12}CH_2{}^{16}OH$ — Continued

| Transition J' K_a' K_c'    J" K_a" K_c" | Freq. obs. (MHz) | Freq. cal. (MHz) | Uncertainty (MHz) | Int. (S) | Energy 'state (cm$^{-1}$) | Ref. |
|---|---|---|---|---|---|---|
| 11( 1 11)− 10( 2  8) |           | 52670.124 |  0.025 | 0.543 | 37.827  |    |
| 11( 2 10)− 10( 3  7) | 53359.400 | 53359.218 |  0.182 | 1.388 | 41.833  | 27 |
|  8( 1  7)−  8( 0  8) |           | 54064.759 |  0.012 | 5.381 | 22.523  |    |
| 12( 3 10)− 13( 0 13) |           | 54641.944 |  0.023 | 0.076 | 53.466  |    |
| 14( 1 14)− 13( 2 11) |           | 54953.271 |  0.031 | 0.333 | 59.515  |    |
| 12( 1 12)− 11( 2  9) |           | 55323.137 |  0.027 | 0.468 | 44.510  |    |
| 13( 1 13)− 12( 2 10) |           | 56061.616 |  0.030 | 0.397 | 51.739  |    |
| 10( 2  8)−  9( 3  7) | 57574.400 | 57574.699 | −0.299 | 1.431 | 36.071  | 27 |
| 18( 8 11)− 19( 7 12) |           | 57652.990 |  0.026 | 1.755 | 155.652 |    |
| 18( 8 10)− 19( 7 13) |           | 57653.568 |  0.026 | 1.755 | 155.652 |    |
| 15( 7  9)− 16( 6 10) | 58279.900 | 58279.976 | −0.076 | 1.422 | 112.796 | 27 |
| 15( 7  8)− 16( 6 11) | 58282.700 | 58282.632 |  0.068 | 1.422 | 112.796 | 27 |
| 28( 2 27)− 27( 3 24) |           | 58778.820 |  0.068 | 0.304 | 235.212 |    |
| 12( 6  7)− 13( 5  8) |           | 58889.539 |  0.011 | 1.091 | 76.936  |    |
| 12( 6  6)− 13( 5  9) |           | 58901.328 |  0.011 | 1.091 | 76.936  |    |
|  2( 1  2)−  1( 0  1) |           | 59297.226 |  0.005 | 1.500 | 2.561   |    |
|  9( 5  5)− 10( 4  6) |           | 59461.837 |  0.012 | 0.761 | 48.073  |    |
|  9( 5  4)− 10( 4  7) |           | 59511.561 |  0.012 | 0.761 | 48.073  |    |
|  6( 4  3)−  7( 3  4) |           | 59943.594 |  0.013 | 0.436 | 26.211  |    |
|  7( 1  6)−  6( 2  5) |           | 59982.342 |  0.011 | 1.390 | 17.727  |    |
|  6( 4  2)−  7( 3  5) |           | 60136.450 |  0.013 | 0.436 | 26.211  |    |
|  3( 3  1)−  4( 2  2) |           | 60214.265 |  0.014 | 0.128 | 11.350  |    |
| 22( 5 18)− 23( 2 21) |           | 60818.987 |  0.034 | 0.156 | 169.966 |    |
|  3( 3  0)−  4( 2  3) |           | 60846.894 |  0.014 | 0.128 | 11.350  |    |
| 27( 2 25)− 28( 1 28) |           | 61138.935 |  0.065 | 0.075 | 227.443 |    |
| 11( 3  9)− 12( 0 12) |           | 61775.990 |  0.022 | 0.064 | 46.441  |    |
| 25( 3 23)− 26( 0 26) |           | 61823.230 |  0.051 | 0.081 | 197.263 |    |
|  9( 1  8)−  9( 0  9) |           | 62407.842 |  0.014 | 5.366 | 27.906  |    |
| 14( 3 12)− 13( 4  9) |           | 62593.444 |  0.012 | 1.857 | 69.268  |    |
| 16( 4 13)− 17( 1 16) |           | 64654.521 |  0.025 | 0.110 | 93.553  |    |
|  9( 2  7)−  9( 1  8) | 65484.589 | 65484.578 |  0.011 | 7.394 | 30.090  | b  |
| 10( 2  8)− 10( 1  9) | 65937.717 | 65937.708 |  0.009 | 8.407 | 36.071  | b  |
|  8( 2  6)−  8( 1  7) |           | 65964.268 |  0.006 | 6.317 | 24.723  |    |
|  5( 0  5)−  4( 1  4) | 65997.178 | 65997.287 | −0.109 | 2.480 | 8.700   | b  |
| 17( 4 14)− 16( 5 11) | 66159.230 | 66159.201 |  0.029 | 2.229 | 103.528 | b  |
| 12( 2 11)− 11( 3  8) | 67140.373 | 67140.405 | −0.032 | 1.483 | 48.769  | b  |
|  7( 2  5)−  7( 1  6) | 67186.574 | 67186.577 | −0.003 | 5.237 | 19.968  | b  |
| 26( 3 24)− 27( 0 27) |           | 67209.221 |  0.056 | 0.077 | 212.274 |    |
| 11( 2  9)− 11( 1 10) | 67485.067 | 67485.049 |  0.018 | 9.295 | 42.664  | b  |
| 20( 5 16)− 19( 6 13) | 67490.834 | 67490.804 |  0.030 | 2.574 | 144.715 | b  |
| 23( 6 18)− 22( 7 15) | 68133.981 | 68134.295 | −0.314 | 2.912 | 192.873 | b  |
| 20( 5 15)− 19( 6 14) | 68328.266 | 68328.266 |  0.000 | 2.576 | 144.742 | b  |
|  6( 2  4)−  6( 1  5) | 68934.899 | 68934.887 |  0.012 | 4.208 | 15.823  | b  |
| 17( 4 13)− 16( 5 12) |           | 69333.517 |  0.011 | 2.240 | 103.631 |    |
| 28( 2 26)− 29( 1 29) |           | 69735.227 |  0.072 | 0.072 | 243.642 |    |
| 27( 2 26)− 26( 3 23) |           | 70251.305 |  0.059 | 0.335 | 219.462 |    |
| 12( 2 10)− 12( 1 11) | 70262.087 | 70262.072 |  0.015 | 10.008 | 49.869 | b  |
| 10( 3  8)− 11( 0 11) |           | 70336.179 |  0.021 | 0.051 | 40.002  |    |
|  5( 2  3)−  5( 1  4) | 70976.836 | 70976.824 |  0.012 | 3.263 | 12.282  | b  |
| 10( 1  9)− 10( 0 10) | 71971.844 | 71971.780 |  0.064 | 5.276 | 33.871  | b  |
| 27( 3 25)− 28( 0 28) |           | 72899.148 |  0.062 | 0.074 | 227.835 |    |
| 14( 3 11)− 13( 4 10) | 73001.994 | 73001.970 |  0.024 | 1.917 | 69.602  | b  |
|  4( 2  2)−  4( 1  3) | 73081.226 | 73081.215 |  0.011 | 2.411 | 9.341   | b  |
| 13( 2 11)− 13( 1 12) | 74380.685 | 74380.662 |  0.023 | 10.516 | 57.682 | b  |
|  3( 1  3)−  2( 0  2) | 74976.055 | 74976.057 | −0.002 | 2.023 | 4.249   | b  |
|  3( 2  1)−  3( 1  2) | 75036.045 | 75036.027 |  0.018 | 1.637 | 6.995   | b  |
| 17( 8 10)− 18( 7 11) |           | 75454.987 |  0.023 | 1.547 | 145.132 |    |
| 17( 8  9)− 18( 7 12) |           | 75455.255 |  0.023 | 1.547 | 145.132 |    |
| 14( 7  8)− 15( 6  9) | 76071.196 | 76071.177 | −0.019 | 1.217 | 104.029 | a  |
| 14( 7  7)− 15( 6 10) | 76072.475 | 76072.388 | −0.087 | 1.217 | 104.029 | a  |
|  2( 2  0)−  2( 1  1) | 76662.495 | 76662.463 |  0.032 | 0.892 | 5.240   | b  |
| 11( 6  6)− 12( 5  7) | 76663.020 | 76662.862 |  0.158 | 0.889 | 69.923  | a  |
| 11( 6  5)− 12( 5  8) | 76668.277 | 76668.117 |  0.160 | 0.889 | 69.923  | a  |
|  8( 5  4)−  9( 4  5) |           | 77213.738 |  0.012 | 0.566 | 42.815  |    |

TABLE 3. Observed and calculated transition frequencies for the ground vibrational state of trans-$^{12}CH_3^{12}CH_2^{16}OH$ — Continued

| Transition J' $K_a'$ $K_c'$   J" $K_a"$ $K_c"$ | Freq. obs. (MHz) | Freq. cal. (MHz) | Uncertainty (MHz) | Int. (S) | 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 $trans$-$^{12}CH_3^{12}CH_2^{16}OH$ — Continued

| Transition J' $K_a'$ $K_c'$ — J'' $K_a''$ $K_c''$ | Freq. obs. (MHz) | Freq. cal. (MHz) | Uncertainty (MHz) | Int. (S) | Energy 'state (cm$^{-1}$) | Ref. |
|---|---|---|---|---|---|---|
| 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-$^{12}CH_3$$^{12}CH_2$$^{16}OH$ — Continued

| J' | $K_a'$ | $K_c'$ | J" | $K_a"$ | $K_c"$ | Freq. obs. (MHz) | Freq. cal. (MHz) | Uncertainty (MHz) | Int. (S) | Energy 'state $(cm^{-1})$ | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 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 | b |
| 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) | | | 155854.475 | 155854.463 | 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*-$^{12}CH_3^{12}CH_2^{16}OH$ — Continued

| Transition $J'$ $K_a'$ $K_c'$ $J''$ $K_a''$ $K_c''$ | Freq. obs. (MHz) | Freq. cal. (MHz) | Uncertainty (MHz) | Int. (S) | Energy 'state (cm⁻¹) | Ref. |
|---|---|---|---|---|---|---|
| 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-$^{12}$CH$_3$$^{12}$CH$_2$$^{16}$OH — Continued

| Transition J' $K_a'$ $K_c'$ — J" $K_a"$ $K_c"$ | Freq. obs. (MHz) | Freq. cal. (MHz) | Uncertainty (MHz) | Int. (S) | Energy 'state (cm⁻¹) | Ref. |
|---|---|---|---|---|---|---|
| 3( 3 0) – 2( 2 1) | 183214.030 | 183213.848 | 0.182 | 2.485 | 11.350 | a |
| 18( 2 17) – 18( 1 18) | 183304.546 | 183304.584 | −0.038 | 4.599 | 102.177 | b |
| 15( 4 12) – 15( 3 13) | 183605.574 | 183605.877 | −0.303 | 8.145 | 84.167 | a |
| 23( 2 21) – 23( 1 22) | 184361.991 | 184361.908 | 0.083 | 9.534 | 167.937 | a |
| 20( 3 18) – 20( 2 19) | 184393.717 | 184393.632 | 0.085 | 8.815 | 130.567 | a |
| 16( 4 13) – 16( 3 14) | 184528.228 | 184528.183 | 0.045 | 8.761 | 93.553 | a |
| 19( 1 18) – 19( 0 19) | 185268.167 | 185268.285 | −0.118 | 4.663 | 112.724 | a |
| 28( 3 26) – 27( 4 23) | | 185543.408 | 0.061 | 1.234 | 243.945 | |
| 17( 4 14) – 17( 3 15) | | 185825.858 | 0.013 | 9.361 | 103.528 | |
| 24( 3 22) – 23( 4 19) | | 185831.393 | 0.030 | 1.989 | 182.807 | |
| 24( 4 21) – 23( 5 18) | | 186644.765 | 0.020 | 3.317 | 189.809 | |
| 18( 4 15) – 18( 3 16) | | 187561.546 | 0.013 | 9.940 | 114.094 | |
| 7( 2 6) – 6( 1 5) | | 188107.573 | 0.012 | 2.735 | 19.798 | |
| 28( 3 25) – 28( 2 26) | | 188750.280 | 0.032 | 14.921 | 249.938 | |
| 27( 3 25) – 26( 4 22) | | 188901.640 | 0.049 | 1.411 | 227.835 | |
| 25( 3 23) – 24( 4 20) | | 189084.772 | 0.035 | 1.799 | 197.264 | |
| 23( 6 18) – 24( 3 21) | | 189561.052 | 0.043 | 0.044 | 192.873 | |
| 19( 3 16) – 18( 4 15) | | 189673.501 | 0.019 | 3.117 | 120.420 | |
| 19( 4 16) – 19( 3 17) | | 189793.754 | 0.014 | 10.491 | 125.248 | |
| 26( 3 24) – 25( 4 21) | | 190105.082 | 0.041 | 1.602 | 212.274 | |
| 11( 1 11) – 10( 0 10) | | 190579.612 | 0.011 | 8.317 | 37.827 | |
| 26( 5 21) – 26( 4 22) | | 190674.898 | 0.034 | 16.785 | 227.894 | |
| 9( 4 6) – 10( 1 9) | | 190901.250 | 0.023 | 0.005 | 40.239 | |
| 16( 5 12) – 17( 2 15) | | 192107.788 | 0.031 | 0.020 | 101.318 | |
| 20( 4 17) – 20( 3 18) | | 192574.664 | 0.015 | 11.008 | 136.991 | |
| 21( 3 19) – 21( 2 20) | | 192602.400 | 0.014 | 8.948 | 142.784 | |
| 13( 1 12) – 12( 2 11) | | 192822.286 | 0.013 | 4.929 | 55.201 | |
| 19( 2 18) – 19( 1 19) | 193791.351 | 193791.411 | −0.060 | 4.619 | 113.022 | a |
| 6( 2 4) – 5( 1 5) | | 195325.481 | 0.012 | .630 | 15.823 | |
| 21( 4 18) – 21( 3 19) | | 195948.255 | 0.015 | 11.486 | 149.320 | |
| 12( 0 12) – 11( 1 11) | | 196458.580 | 0.010 | 9.233 | 44.381 | |
| 25( 5 20) – 25( 4 21) | | 197172.160 | 0.028 | 15.616 | 212.510 | |
| 20( 1 19) – 20( 0 20) | | 197939.372 | 0.021 | 4.662 | 124.188 | |
| 16( 10 6) – 17( 9 9) | | 197975.287 | 0.073 | 0.840 | 166.526 | |
| 16( 10 7) – 17( 9 8) | | 197975.287 | 0.073 | 0.840 | 166.526 | |
| 13( 9 5) – 14( 8 6) | | 198547.523 | 0.019 | 0.547 | 123.709 | |
| 13( 9 4) – 14( 8 7) | | 198547.523 | 0.019 | 0.547 | 123.709 | |
| 24( 2 22) – 24( 1 23) | | 198644.410 | 0.021 | 9.463 | 182.019 | |
| 10( 8 3) – 11( 7 4) | | 199065.704 | 0.018 | 0.279 | 87.884 | |
| 10( 8 2) – 11( 7 5) | | 199065.704 | 0.018 | 0.279 | 87.884 | |
| 23( 4 19) – 22( 5 18) | | 199145.199 | 0.022 | 3.460 | 176.609 | |
| 7( 7 1) – 8( 6 2) | | 199520.617 | 0.022 | 0.064 | 59.054 | |
| 7( 7 0) – 8( 6 3) | | 199520.617 | 0.022 | 0.064 | 59.054 | |
| 22( 4 19) – 22( 3 20) | | 199948.815 | 0.016 | 11.920 | 162.234 | |
| 16( 2 14) – 15( 3 13) | | 200121.992 | 0.017 | 3.555 | 84.718 | |
| 4( 3 2) – 3( 2 1) | | 200569.534 | 0.013 | 2.579 | 13.686 | |
| 4( 3 1) – 3( 2 2) | | 200787.380 | 0.013 | 2.577 | 13.686 | |
| 22( 3 20) – 22( 2 21) | | 201331.510 | 0.015 | 9.053 | 155.565 | |
| 8( 2 7) – 7( 1 6) | | 201437.332 | 0.012 | 3.088 | 24.446 | |
| 25( 4 22) – 24( 5 19) | | 201590.968 | 0.024 | 3.369 | 204.465 | |
| 24( 5 19) – 24( 4 20) | | 203384.064 | 0.023 | 14.562 | 197.741 | |
| 29( 3 26) – 29( 2 27) | | 203854.869 | 0.038 | 14.680 | 267.170 | |
| 20( 2 19) – 20( 1 20) | | 204495.550 | 0.021 | 4.634 | 124.416 | |
| 23( 4 20) – 23( 3 21) | | 204599.863 | 0.016 | 12.309 | 175.732 | |
| 12( 1 12) – 11( 0 11) | | 205458.497 | 0.011 | 9.325 | 44.510 | |
| 23( 5 18) – 23( 4 19) | 209100.261 | 209100.137 | 0.124 | 13.608 | 183.584 | |
| 24( 4 21) – 24( 3 22) | | 209913.509 | 0.017 | 12.650 | 189.809 | |
| 21( 1 20) – 21( 0 21) | 210391.112 | 210391.175 | −0.063 | 4.663 | 136.186 | b |
| 23( 3 21) – 23( 2 22) | 210532.832 | 210532.745 | 0.087 | 9.135 | 168.907 | a |
| 8( 4 5) – 9( 1 8) | | 211983.020 | 0.025 | 0.002 | 34.977 | |
| 25( 2 23) – 25( 1 24) | 212746.107 | 212746.056 | 0.051 | 9.420 | 196.631 | a |
| 13( 0 13) – 12( 1 12) | 213856.261 | 213856.270 | −0.009 | 10.282 | 51.643 | a |
| 22( 5 17) – 22( 4 18) | 214180.117 | 214179.975 | 0.142 | 12.736 | 170.034 | a |
| 9( 2 8) – 8( 1 7) | 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*-$^{12}CH_3{}^{12}CH_2{}^{16}OH$ — Continued

| Transition J' Ka' Kc' | J" Ka" Kc" | Freq. obs. (MHz) | Freq. cal. (MHz) | Uncertainty (MHz) | Int. (S) | Energy 'state (cm$^{-1}$) | Ref. |
|---|---|---|---|---|---|---|---|
| 14( 1 13) – | 13( 2 12) | 214699.879 | 214699.859 | 0.020 | 5.805 | 63.431 | a |
| 21( 2 20) – | 21( 1 21) | 215375.642 | 215375.682 | −0.040 | 4.646 | 136.359 | b |
| 26( 4 23) – | 25( 5 20) | 215452.238 | 215452.202 | 0.036 | 3.379 | 219.696 | a |
| 20( 3 17) – | 19( 4 16) | | 215610.762 | 0.020 | 3.428 | 132.440 | |
| 25( 4 22) – | 25( 3 23) | 215890.440 | 215890.261 | 0.179 | 12.944 | 204.465 | a |
| 12( 9 4) – | 13( 8 5) | 216127.000 | 216126.776 | 0.224 | 0.393 | 116.117 | a |
| 12( 9 3) – | 13( 8 6) | 216127.000 | 216126.776 | 0.224 | 0.393 | 116.117 | a |
| 9( 8 2) – | 10( 7 3) | 216625.420 | 216625.442 | −0.022 | 0.154 | 82.045 | a |
| 9( 8 1) – | 10( 7 4) | 216625.420 | 216625.442 | −0.022 | 0.154 | 82.045 | a |
| 15( 5 11) – | 16( 2 14) | | 216699.408 | 0.030 | 0.013 | 84.718 | |
| 22( 6 17) – | 23( 3 20) | | 217392.407 | 0.039 | 0.032 | 172.132 | |
| 5( 3 3) – | 4( 2 2) | 217803.689 | 217803.699 | −0.010 | 2.714 | 16.607 | a |
| 5( 3 2) – | 4( 2 3) | 218461.226 | 218461.187 | 0.039 | 2.706 | 16.607 | a |
| 21( 5 16) – | 21( 4 17) | 218554.499 | 218554.391 | 0.108 | 11.926 | 157.087 | a |
| 7( 2 5) – | 6( 1 6) | 218654.081 | 218654.042 | 0.039 | 1.550 | 19.968 | a |
| 24( 3 22) – | 24( 2 23) | 220154.784 | 220154.693 | 0.091 | 9.198 | 182.807 | a |
| 13( 1 13) – | 12( 0 12) | 220601.927 | 220601.945 | −0.018 | 10.344 | 51.739 | a |
| 20( 5 15) – | 20( 4 16) | 222217.285 | 222217.201 | 0.084 | 11.164 | 144.742 | a |
| 26( 4 23) – | 26( 3 24) | 222519.499 | 222519.281 | 0.218 | 13.193 | 219.696 | a |
| 22( 1 21) – | 22( 0 22) | 222644.166 | 222644.229 | −0.063 | 4.665 | 148.719 | b |
| 24( 4 20) – | 23( 5 19) | 224119.273 | 224119.480 | −0.207 | 3.676 | 190.957 | a |
| 19( 5 14) – | 19( 4 15) | 225210.356 | 225210.293 | 0.063 | 10.435 | 132.995 | a |
| 17( 2 15) – | 16( 3 14) | 225229.250 | 225229.272 | −0.022 | 4.102 | 94.910 | a |
| 22( 2 21) – | 22( 1 22) | 226395.490 | 226395.538 | −0.048 | 4.654 | 148.849 | b |
| 26( 2 24) – | 26( 1 25) | 226581.339 | 226581.326 | 0.013 | 9.394 | 211.773 | a |
| 10( 2 9) – | 9( 1 8) | 226661.701 | 226661.750 | −0.049 | 3.938 | 35.466 | a |
| 18( 5 13) – | 18( 4 14) | 227606.079 | 227606.064 | 0.015 | 9.732 | 121.843 | a |
| 27( 4 24) – | 26( 5 21) | 228005.820 | 228005.817 | 0.003 | 3.342 | 235.499 | a |
| 17( 5 12) – | 17( 4 13) | 229491.131 | 229491.134 | −0.003 | 9.048 | 111.286 | a |
| 27( 4 24) – | 27( 3 25) | 229779.303 | 229779.075 | 0.228 | 13.400 | 235.499 | a |
| 25( 3 23) – | 25( 2 24) | 230144.820 | 230144.733 | 0.087 | 9.245 | 197.264 | a |
| 16( 5 11) – | 16( 4 12) | 230953.778 | 230953.788 | −0.010 | 8.379 | 101.321 | a |
| 14( 0 14) – | 13( 1 13) | 230991.374 | 230991.382 | −0.008 | 11.325 | 59.444 | a |
| 21( 5 17) – | 21( 4 18) | 231558.549 | 231558.511 | 0.038 | 11.670 | 157.044 | a |
| 20( 5 16) – | 20( 4 17) | 231560.901 | 231560.878 | 0.023 | 11.003 | 144.715 | a |
| 19( 5 15) – | 19( 4 16) | 231737.606 | 231737.595 | 0.011 | 10.337 | 132.978 | a |
| 22( 5 18) – | 22( 4 19) | 231790.000 | 231789.994 | 0.006 | 12.332 | 169.966 | a |
| 18( 5 14) – | 18( 4 15) | 232034.630 | 232034.632 | −0.002 | 9.673 | 121.833 | a |
| 15( 5 10) – | 15( 4 11) | 232075.832 | 232075.861 | −0.029 | 7.721 | 91.948 | a |
| 23( 5 19) – | 23( 4 20) | 232318.499 | 232318.457 | 0.042 | 12.985 | 183.481 | a |
| 17( 5 13) – | 17( 4 14) | 232404.808 | 232404.845 | −0.037 | 9.013 | 111.280 | a |
| 16( 5 12) – | 16( 4 13) | 232808.832 | 232808.877 | −0.045 | 8.359 | 101.318 | a |
| 14( 5 9) – | 14( 4 10) | 232928.499 | 232928.546 | −0.047 | 7.072 | 83.165 | a |
| 14( 10 5) – | 15( 9 6) | 233147.883 | 233147.983 | −0.100 | 0.511 | 148.423 | a |
| 14( 10 4) – | 15( 9 7) | 233147.883 | 233147.983 | −0.100 | 0.511 | 148.423 | a |
| 7( 4 4) – | 8( 1 7) | | 233187.274 | 0.027 | 0.001 | 30.301 | |
| 24( 5 20) – | 24( 4 21) | 233208.521 | 233208.512 | 0.009 | 13.623 | 197.588 | a |
| 15( 5 11) – | 15( 4 12) | 233215.475 | 233215.523 | −0.048 | 7.710 | 91.946 | a |
| 13( 5 8) – | 13( 4 9) | 233571.024 | 233571.071 | −0.047 | 6.430 | 74.971 | a |
| 14( 5 10) – | 14( 4 11) | 233601.523 | 233601.578 | −0.055 | 7.066 | 83.164 | a |
| 13( 5 9) – | 13( 4 10) | 233951.119 | 233951.252 | −0.133 | 6.427 | 74.971 | a |
| 12( 5 7) – | 12( 4 8) | 234051.119 | 234051.162 | −0.043 | 5.790 | 67.366 | a |
| 8( 8 1) – | 9( 7 2) | 234169.691 | 234169.777 | −0.086 | 0.057 | 76.791 | a |
| 8( 8 0) – | 9( 7 3) | 234169.691 | 234169.777 | −0.086 | 0.057 | 76.791 | a |
| 12( 5 8) – | 12( 4 9) | 234255.161 | 234255.255 | −0.094 | 5.789 | 67.366 | b |
| 11( 5 6) – | 11( 4 7) | 234406.451 | 234406.436 | 0.015 | 5.151 | 60.348 | a |
| 11( 5 7) – | 11( 4 8) | 234509.565 | 234509.671 | −0.106 | 5.151 | 60.348 | b |
| 25( 5 21) – | 25( 4 22) | 234523.893 | 234523.936 | −0.043 | 14.241 | 212.288 | a |
| 10( 5 5) – | 10( 4 6) | 234666.273 | 234666.132 | 0.141 | 4.508 | 53.918 | a |
| 10( 5 6) – | 10( 4 7) | 234714.571 | 234714.773 | −0.202 | 4.508 | 53.918 | b |
| 23( 1 22) – | 23( 0 23) | 234725.600 | 234725.664 | −0.064 | 4.668 | 161.788 | b |
| 6( 3 4) – | 5( 2 3) | 234758.820 | 234758.825 | −0.005 | 2.864 | 20.113 | a |
| 9( 5 4) – | 9( 4 5) | 234853.026 | 234852.837 | 0.189 | 3.856 | 48.073 | a |
| 9( 5 5) – | 9( 4 6) | 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*-$^{12}CH_3{}^{12}CH_2{}^{16}OH$ — Continued

| Transition J' $K_a'$ $K_c'$   J" $K_a''$ $K_c''$ | Freq. obs. (MHz) | Freq. cal. (MHz) | Uncertainty (MHz) | Int. (S) | 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*-$^{12}CH_3{}^{12}CH_2{}^{16}OH$ — Continued

| Transition | | | | | Freq. obs. (MHz) | Freq. cal. (MHz) | Uncertainty (MHz) | Int. (S) | Energy 'state (cm$^{-1}$) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|
| J' | $K_a'$ $K_c'$ | | J" | $K_a"$ $K_c"$ | | | | | | |
| 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*-$^{12}CH_3^{12}CH_2^{16}OH$ — Continued

| J' | $K_a'$ | $K_c'$ | J" | $K_a"$ | $K_c"$ | Freq. obs. (MHz) | Freq. cal. (MHz) | Uncertainty (MHz) | Int. (S) | Energy 'state (cm⁻¹) | Ref. |
|----|----|----|----|----|----|----|----|----|----|----|----|
| 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*-$^{12}CH_3{}^{12}CH_2{}^{16}OH$ — Continued

| Transition J' $K_a'$ $K_c'$  J" $K_a"$ $K_c"$ | Freq. obs. (MHz) | Freq. cal. (MHz) | Uncertainty (MHz) | Int. (S) | Energy 'state (cm$^{-1}$) | Ref. |
|---|---|---|---|---|---|---|
| 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 | 0.568 | 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*-$^{12}CH_3^{12}CH_2^{16}OH$ — Continued

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

TABLE 3. Observed and calculated transition frequencies for the ground vibrational state of *trans*-$^{12}CH_3^{12}CH_2^{16}OH$ — Continued

| Transition J' $K_a'$ $K_c'$ — J" $K_a"$ $K_c"$ | Freq. obs. (MHz) | Freq. cal. (MHz) | Uncertainty (MHz) | Int. (S) | Energy 'state (cm$^{-1}$) | Ref. |
|---|---|---|---|---|---|---|
| 9( 7 2)- 8( 6 3) | | 497087.805 | 0.021 | 6.599 | 68.980 | |
| 12( 6 7)- 11( 5 6) | | 497275.403 | 0.018 | 6.141 | 76.936 | |
| 12( 6 6)- 11( 5 7) | | 497277.641 | 0.018 | 6.141 | 76.936 | |
| 13( 3 11)- 12( 0 12) | | 500490.036 | 0.024 | 0.161 | 61.075 | |
| 7( 4 4)- 6( 1 5) | | 502978.274 | 0.029 | 0.002 | 30.301 | |
| 30( 1 29)- 29( 2 28) | | 504321.951 | 0.059 | 22.552 | 268.326 | |
| 21( 4 18)- 20( 3 17) | | 506048.815 | 0.028 | 5.767 | 149.320 | |
| 16( 2 14)- 15( 1 15) | | 506128.092 | 0.033 | 0.412 | 84.718 | |
| 6( 4 2)- 5( 1 5) | | 506763.669 | 0.031 | 0.001 | 26.211 | |
| 18( 4 14)- 17( 3 15) | | 507291.511 | 0.021 | 4.621 | 114.251 | |
| 31( 0 31)- 30( 1 30) | | 509452.731 | 0.070 | 28.544 | 274.762 | |
| 16( 5 12)- 15( 4 11) | | 512987.422 | 0.018 | 5.883 | 101.318 | |
| 18( 7 12)- 19( 4 15) | | 513617.604 | 0.035 | 0.003 | 142.615 | |
| 18( 3 15)- 17( 2 16) | | 513620.524 | 0.026 | 1.853 | 109.016 | |
| 16( 5 11)- 15( 4 12) | | 514268.482 | 0.018 | 5.873 | 101.321 | |
| 10( 7 4)- 9( 6 3) | | 514580.636 | 0.021 | 6.701 | 74.820 | |
| 10( 7 3)- 9( 6 4) | | 514580.638 | 0.021 | 6.701 | 74.820 | |
| 22( 4 19)- 21( 3 18) | | 514589.277 | 0.031 | 6.039 | 162.234 | |
| 13( 6 8)- 12( 5 7) | | 514694.032 | 0.018 | 6.288 | 84.534 | |
| 13( 6 7)- 12( 5 8) | | 514699.469 | 0.018 | 6.288 | 84.534 | |
| 8( 4 5)- 7( 1 6) | | 517123.248 | 0.027 | 0.004 | 34.977 | |
| 23( 4 20)- 22( 3 19) | | 522514.098 | 0.035 | 6.371 | 175.732 | |
| 32( 0 32)- 31( 1 31) | | 525662.017 | 0.082 | 29.548 | 292.297 | |
| 14( 3 12)- 13( 0 13) | | 528381.227 | 0.025 | 0.180 | 69.268 | |
| 7( 4 3)- 6( 1 6) | | 528421.472 | 0.029 | 0.001 | 30.301 | |
| 19( 4 15)- 18( 3 16) | | 528991.059 | 0.022 | 4.487 | 125.482 | |
| 17( 5 13)- 16( 4 12) | | 529517.834 | 0.019 | 6.000 | 111.280 | |
| 24( 4 21)- 23( 3 20) | | 529964.513 | 0.039 | 6.772 | 189.809 | |
| 9( 4 6)- 8( 1 7) | | 531116.387 | 0.025 | 0.007 | 40.239 | |
| !7( 5 12)- 16( 4 13) | | 531633.529 | 0.019 | 5.982 | 111.286 | |
| 8( 8 0)- 7( 7 1) | | 531736.964 | 0.027 | 7.487 | 76.791 | |
| 8( 8 1)- 7( 7 0) | | 531736.964 | 0.027 | 7.487 | 76.791 | |
| 11( 7 5)- 10( 6 4) | | 532066.084 | 0.021 | 6.820 | 81.244 | |
| 11( 7 4)- 10( 6 5) | | 532066.092 | 0.021 | 6.820 | 81.244 | |
| 14( 6 9)- 13( 5 8) | | 532080.491 | 0.019 | 6.435 | 92.719 | |
| 14( 6 8)- 13( 5 9) | | 532092.722 | 0.019 | 6.435 | 92.719 | |
| 17( 7 11)- 18( 4 14) | | 534746.458 | 0.034 | 0.002 | 132.088 | |
| 25( 4 22)- 24( 3 21) | | 537093.902 | 0.045 | 7.251 | 204.465 | |
| 26( 4 23)- 25( 3 22) | | 544066.189 | 0.051 | 7.813 | 219.696 | |
| 10( 4 7)- 9( 1 8) | | 545102.708 | 0.024 | 0.013 | 46.088 | |
| 18( 5 14)- 17( 4 13) | | 545695.881 | 0.020 | 6.107 | 121.833 | |
| 17( 2 15)- 16( 1 16) | | 545906.607 | 0.033 | 0.357 | 94.910 | |
| 19( 3 16)- 18( 2 17) | | 546937.218 | 0.028 | 1.613 | 120.420 | |
| 18( 5 13)- 17( 4 14) | | 549071.717 | 0.020 | 6.076 | 121.843 | |
| 9( 8 1)- 8( 7 2) | | 549238.936 | 0.025 | 7.517 | 82.045 | |
| 9( 8 2)- 8( 7 1) | | 549238.936 | 0.025 | 7.517 | 82.045 | |
| 15( 6 10)- 14( 5 9) | | 549426.546 | 0.020 | 6.582 | 101.492 | |
| 15( 6 9)- 14( 5 10) | | 549452.342 | 0.020 | 6.582 | 101.492 | |
| 12( 7 6)- 11( 6 5) | | 549541.517 | 0.021 | 6.951 | 88.254 | |
| 12( 7 5)- 11( 6 6) | | 549541.544 | 0.021 | 6.951 | 88.254 | |
| 8( 4 4)- 7( 1 7) | | 550960.082 | 0.028 | 0.002 | 34.977 | |
| 20( 4 16)- 19( 3 17) | | 551989.357 | 0.024 | 4.298 | 137.330 | |
| 16( 7 10)- 17( 4 13) | | 555151.256 | 0.032 | 0.001 | 122.149 | |
| 15( 3 13)- 14( 0 14) | | 557572.571 | 0.027 | 0.194 | 78.043 | |
| 11( 4 8)- 10( 1 9) | | 559252.498 | 0.024 | 0.022 | 52.526 | |
| 19( 5 15)- 18( 4 14) | | 561419.623 | 0.021 | 6.203 | 132.978 | |
| 19( 5 14)- 18( 4 15) | | 566639.806 | 0.021 | 6.153 | 132.995 | |
| 16( 6 11)- 15( 5 10) | | 566722.081 | 0.020 | 6.726 | 110.852 | |
| 10( 8 2)- 9( 7 3) | | 566738.281 | 0.025 | 7.584 | 87.884 | |
| 10( 8 3)- 9( 7 2) | | 566738.281 | 0.025 | 7.584 | 87.884 | |
| 16( 6 10)- 15( 5 11) | | 566773.577 | 0.020 | 6.725 | 110.852 | |
| 13( 7 7)- 12( 6 6) | | 567003.953 | 0.022 | 7.090 | 95.849 | |
| 13( 7 6)- 12( 6 7) | | 567004.032 | 0.022 | 7.090 | 95.849 | |
| 12( 4 9)- 11( 1 10) | | 573760.599 | 0.024 | 0.035 | 59.552 | |

TABLE 3. Observed and calculated transition frequencies for the ground vibrational state of *trans*-$^{12}CH_3^{12}CH_2^{16}OH$ — Continued

| Transition $J'$ $K_a'$ $K_c'$ $J''$ $K_a''$ $K_c''$ | Freq. obs. (MHz) | Freq. cal. (MHz) | Uncertainty (MHz) | Int. (S) | Energy 'state (cm$^{-1}$) | Ref. |
|---|---|---|---|---|---|---|
| 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 (MHz) | Uncert. (1σ) | Lovas ref. [27] (MHz) | Uncert. (1σ) |
|---|---|---|---|---|
| $A$ | 34891.7707 | (40) | 34891.7542 | (197) |
| $B$ | 9350.6776 | (6) | 9350.6752 | (61) |
| $C$ | 8135.2352 | (3) | 8135.2313 | (58) |
| $\Delta_J$ | 0.00853736 | (76) | 0.0085523 | (749) |
| $\Delta_{JK}$ | −0.0287785 | (300) | −0.028410 | (677) |
| $\Delta_K$ | 0.252460 | (120) | 0.251542 | (488) |
| $\delta_J$ | 0.00173766 | (46) | 0.0017397 | (106) |
| $\delta_K$ | 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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