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Searching for trans ethyl methyl ether in Orion KL★,★★

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Abstract

We report on the tentative detection of trans ethyl methyl ether (tEME), t-$CH_3CH_2OCH_3$, through the identification of a large number of rotational lines from each one of the spin states of the molecule towards Orion KL. We also search for gauche-trans-n-propanol, Gt-n-$CH_3CH_2CH_2OH$, an isomer of tEME in the same source. We have identified lines of both species in the IRAM 30 m line survey and in the ALMA Science Verification data. We have obtained ALMA maps to establish the spatial distribution of these species. Whereas tEME mainly arises from the compact ridge component of Orion, Gt-n-propanol appears at the emission peak of ethanol (south hot core). The derived column densities of these species at the location of their emission peaks are $\leq(4.0 \pm 0.8) \times 10^{15}$ cm^{-2} and $\leq(1.0 \pm 0.2)\times 10^{15}$ cm^{-2} for tEME and Gt-n-propanol, respectively. The rotational temperature is ~100 K for both molecules. We also provide maps of CH_3OCOH, CH_3CH_2OCOH, CH_3OCH_3, CH_3OH, and CH_3CH_2OH to compare the distribution of these organic saturated O-bearing species containing methyl and ethyl groups in this region. Abundance

★This paper makes use of the following ALMA data: ADS/JAO.ALMA#2011.0.00009.SV. ALMA is a partnership of ESO (representing its member states), NSF (USA), and NINS (Japan) with NRC (Canada), NSC, and ASIAA (Taiwan), and KASI (Republic of Korea), in cooperation with the Republic of Chile. The Joint ALMA Observatory is operated by ESO, AUI/NRAO, and NAOJ. This work was also based on observations carried out with the IRAM 30-m telescope. IRAM is supported by INSU/CNRS (France), MPG (Germany), and IGN (Spain).

★★Appendix A is available in electronic form at http://www.aanda.org

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ratios of related species and upper limits to the abundances of non-detected ethers are provided. We derive an abundance ratio $N(CH_3OCH_3)/N(\text{tEME}) \geq 150$ in the compact ridge of Orion.

Keywords

ISM: abundances; ISM: clouds; ISM: individual objects: Orion KL; ISM: molecules; radio lines: ISM; surveys

1. Introduction

The spectral millimeter-wave survey of Orion KL carried out with the IRAM 30 m radio telescope (Tercero et al. 2010; Tercero 2012) shows more than 15 400 spectral features of which about 11 000 have been identified and attributed to 50 molecules (199 different isotopologues and vibrational modes). To date, there have been several works based on these data. As the result of a fruitful collaboration with spectroscopy laboratories, 3000 previously unidentified lines have been assigned to new species in the interstellar medium (ISM). We have detected in space 16 new isotopologues and vibrationally excited states of abundant molecules in Orion for the first time (Demyk et al. 2007; Margulès et al. 2009, 2010; Carvajal et al. 2009; Tercero et al. 2012; Motiyenko et al. 2012; Daly et al. 2013; Coudert et al. 2013; Haykal et al. 2014; López et al. 2014) as well as four new molecules (Tercero et al. 2013; Cernicharo et al. 2013; Kolesniková et al. 2014). These identifications reduce the number of unidentified lines and mitigate line confusion in the spectra. Nevertheless, many features still remain unidentified and correspond to new species that we have to search and identify. Formates, ethers, acetates, alcohols, and cyanides are the best candidates for this purpose in Orion.

The recent search for trans ethyl methyl ether (tEME) in selected hot cores (Sgr B2(N-LMH) and W51 e1/e2) by Carroll et al. (2015) only provides upper limits to tEME. Hence, the results from that work do not confirm the previous tentative identification of this species by Fuchs et al. (2005) towards W51 e1/e2.

A systematic line survey with most weeds removed permits us to address the problem of the abundances of isomers and derivatives of key species, such as methyl formate (A. López et al., in prep.), through combined IRAM and ALMA studies.

In this Letter, we report on the tentative detection of tEME towards the compact ridge (CR) of Orion KL. We have detected emission of features arising from the five spin states at 3, 2, and 1 mm with the IRAM 30 m telescope and the ALMA interferometer. In addition, several unidentified lines of these data have been identified as belonging to the gauche-trans conformer of n-propanol (an isomer of tEME). ALMA maps of organic saturated O-bearing species containing methyl, ethyl, and propyl groups, abundance ratios of related species, and upper limits to the column densities of non-detected ethers are presented and discussed in Sect. 4.

2. Observations

IRAM 30 m: new data of the IRAM 30 m telescope, which complement and improve those of Tercero et al. (2010), were collected in August 2013 and March 2014 towards Orion KL (see Tercero et al. 2010 and López et al. 2014, for information about the previous data set). Frequencies in the ranges 80.7–116, 122.7–161.2, 199.7–291.0, 291.4–306.7GHz, were observed with the EMIR receivers connected to the FFTS (200 kHz of spectral resolution) spectrometers. We pointed towards IRc2 source at $\alpha_{2000.0} = 5^h35^m\ 14^s.5$, $\delta_{2000.0} = -5°22'30''.0$, corresponding to the survey position (see Sect. 4). We observed an additional position to target the CR: $\alpha_{2000.0} = 5^h35^m14^s.3$, $\delta_{2000.0} = -5°22'37''.0$ (see Sect. 4). The observations were performed using the wobbler switching mode with a beam throw in azimuth of ±120″. The intensity scale was calibrated using the atmospheric transmission model (ATM, Cernicharo 1985; Pardo et al. 2001). Focus and pointing were checked every 1–2 h on planets or nearby quasars. System temperatures were in the range of 100–800 K from the lowest to highest frequencies. Half power beam width (HPBW) ranged from 31″ to 8″ from 80 to 307 GHz (*HPBW*[arcsec] = 2460/Freq.[GHz]). The data were reduced using the GILDAS package[1].

ALMA SV: the ALMA Science Verification (SV) data[2] were taken in January 2012 towards the IRc2 region in Orion. The observations were carried out with 16 antennas of 12 m in Band 6 (213.715–246.627GHz). The primary beam was ≃27″. Spectral resolution was 0.488 MHz corresponding to a velocity resolution of 0.64 km s^{-1}. The observations were centred on coordinates: $\alpha_{J2000} = 05^h35^m14^s.35$, $\delta_{J2000} = -05°22'35''.00$. The CASA software[3] was used for initial processing and then the visibilities were exported to the GILDAS package. The line maps were cleaned using the HOGBOM algorithm (Högbom 1974). The synthesized beam ranged from 2″.00 × 1″.48 with a PA of 176° at 214.0 GHz to 1″.75 × 1″. 29 with a PA of 164× at 246.4 GHz. The brightness temperature to flux density conversion factor is 9 K for 1 Jy per beam.

3. Results

3.1. Search for trans ethyl methyl ether

ALMA SV data: frequency predictions from Fuchs et al. (2003) and dipole moments measured by Hayashi & Kuwada (1975) of tEME were implemented in MADEX (Cernicharo 2012) to model the emission of this species and search for it towards Orion KL. Using the ALMA SV data, we extracted the averaged spectrum over 5 × 5 pixels (1″ × 1″) around the CH_3OCH_3 emission peak of the CR component (Position A; see Sect. 4). The advantage of ALMA with respect to single dish telescope data (see below) is the drastic reduction of the confusion limit. The ALMA SV data show the presence of tEME as shown in Fig. 1 (selected lines) and Fig. A.1 (all lines favourable for detection (corresponding to *b*-type transitions with upper level energies up to 300 K and large line strenghts, $S_{ij} \geq 1$) present in the ALMA SV frequency range). The model that best fits the data is shown with

[1]http://www.iram.fr/IRAMFR/GILDAS
[2]http://almascience.eso.org/almadata/sciver/OrionKLBand6/
[3]http://casa.nrao.edu

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the red line. The assumed parameters are a source size of 3″, v_{LSR} = +7.5 km s^{-1}, Δv = 2.0 km s^{-1}, and T_K = 100 ± 20 K. Using MADEX and assuming local thermodynamic equilibrium (LTE), we obtain $N_{g.s.}$(tEME) ≤ (4.0 ± 0.8) × 10^{15} cm^{-2}. In our models, rotation temperature and column density values are given with their corresponding uncertainty and we obtained them by fitting all available lines by eye. We adopted the source size in agreement with the emission of the maps (see below). In addition, a considerable number of unblended features allows us to fix the radial velocities and line widths. According to our model, in the ALMA frequency range only 33% of the detectable lines of tEME (102 lines) are totally hidden by the emission of stronger lines of other species. At least 46 lines (45% of the detectable lines) shown in Fig. A.1 are free of blending, i.e. these lines are present at the expected radial velocity and there are no other species with significant intensity at the same observed frequency (±3 MHz). Another point to ensure this tentative detection is that the forest of lines emitted by tEME between 215.5 and 215.7 GHz is not covered by lines of abundant molecules in the source allowing the detection of several lines that follow a straightened pattern (see Fig. 1). Hence, there are several clues that could reveal the presence of this species in the CR of Orion KL, but further analysis exploring new available ALMA data and modelling all the molecular content of the CR is needed to give the definitive detection in space of tEME. Table A.1 gives line parameters and blends of all lines of favourable transitions in the ALMA SV data. The spatial distribution of tEME is shown in Fig. 2. Lines that we found to be unblended at the Position A appear blended with emission from other components in the averaged spectrum (see the case of the 30 m data). We selected a line at 245.274 GHz, which is mixed with some emission from extreme velocities of $^{34}SO_2$ and SO_2. Nevertheless, the emission of tEME at Position A in Fig. 2 is not blended (see Sect. 4).

IRAM 30 m data: to search for tEME in the IRAM data, a synthetic spectra of tEME (red curve in Fig. A.2) was obtained with MADEX assuming LTE and adopting the following physical parameters: source diameter 3″, T_K = 100 ± 30 K, v_{LSR} = +7.5 km s^{-1}, Δv = 1.5 km s^{-1}; and a column density of (9±3)×10^{15} cm^{-2} for the ground state (g.s.) of tEME. According to our model, all favourable lines for detection in the 30 m data were detected or were blended with features from more abundant species. Nevertheless, owing to the weakness of the features (T_{MB} < 0.1 K at 3 mm, T_{MB} < 0.2 K at 2 mm, and T_{MB} < 1 K at 1.3–0.9 mm) and the high level of line confusion at ~1 mm, only a few lines were mostly free of blending with other species in this domain. Whereas the synthetic beam of the ALMA SV is 1″.90 × 1″.40, in the 30 m the beam diameter ranging from 30″ to 8″. Therefore, in the 30 m data, the spectrum is a mix of all molecules from all source components (average spectrum over the beam) given rise to a high level of line blending and line confusion. Table A.2 shows line parameters, intensity provided by the model, and blends of all lines of favourable transitions in the 30 m data.

3.2. Search for gauche-trans-n-propanol

All lines of Gt-$CH_3CH_2CH_2OH$, an isomer of C_3H_8O (as well as tEME), reported by Maeda et al. (2006) and the dipole moments from Abdurakhmanov et al. (1969) were used to derive its rotational constants and to implement this species in MADEX. We conducted the search for Gt-n-propanol in the ALMA SV data at two different positions: Position A and the position where the emission peak of ethanol is located (Position B; see Sect. 4). We assign several unidentified lines in the source at Position B to this species. According to our model (d_{sou} = 3″, v_{LSR} = +8.0 km s^{-1}, Δv = 3.0 km s^{-1}, T_K = 100 ± 20 K, and $N_{g.s}$ ≤ (1.0 ± 0.2) × 10^{15} cm^{-2}), many of the lines are below the detection limit although the strongest features are detected. Unfortunately, several lines remain blended (see Fig. A.3). A few lines of this species are also detected in the IRAM 30 m data at the survey position (Fig. A.2 bottom panel; model parameters: d_{sou} = 3″, v_{LSR} = +8.0 km s^{-1}, Δv = 1.5 km s^{-1}, T_K = 100 ± 20 K, and $N_{g.s}$ ≤ (2.0 ± 0.4) × 10^{15} cm^{-2}). Table A.3 shows line parameters for the detected lines. The derived upper limit to its column density (assuming the same physical parameters than those of the tEME ALMA model) at Position A is ≤(3.0 ± 0.6) × 10^{14} cm^{-2}. The spatial distribution of this species around Position B is shown in Fig. 2. To perform the ALMA map, we averaged the emission between v_{LSR} 6 and 9 km s^{-1} of two lines (lines at 236.138 and 244.765GHz). Emission around source *I* should be due to other less abundant species in Orion (we did not find Gt-n-propanol at these positions).

4. Discussion

Species containing the functional groups formate, alcohol, and ether have been detected in Orion with both the methyl and ethyl groups (methyl formate (MF), ethyl formate (EF), methanol, ethanol, dimethyl ether (DME), and tEME). ALMA maps for the spatial distribution of these species as well as Gt-n-propanol are shown in Fig. 2. To address the flux filtered out by ALMA and the accuracy of the maps in a larger energy range, the following discussion is also based on the maps shown in Fig. 5 of Feng et al. (2015; maps performed mixing SMA and IRAM 30 m data) with MF, DME, methanol, and ethanol. For MF, DME, and methanol the spatial distribution and the position of the emission peaks are in agreement with those of the maps presented in this work (note, however, that the ALMA maps provide a more detailed structure at small scales, i.e. ≤5″). For ethanol, we note a more extended spatial distribution in the map of Feng et al. (2015) mostly due to the lower energy of the transition involved. Nevertheless, the emission peak of ethanol is located at the same position.

For the methyl species, we note: i) a rather similar spatial structure: the three species present the V shape distribution of several clumps (at least six) studied by Favre et al. (2011) for the distribution of MF, which was mapped using data from the Plateau de Bure Interferometer (PdBI); ii) that although Brouillet et al. (2013) probed a striking similarity between the spatial distributions of CH_3OCH_3 and CH_3OCOH, we found some differences in the relative intensities of both species. These differences could be mostly due to different excitation temperatures of the involved transitions; and iii) although methanol also follows this V shape structure, a displacement of the intensity peaks is observed with respect to MF. This behaviour suggests methanol as a possible precursor of MF and DME (see also Neill et al. 2011).

Comparing the methyl and ethyl species, we note: i) a reduced spatial distribution of the three ethyl species with respect to their methyl counterpart; ii) the two emission peaks of EF are correlated with those found in MF; iii) the emission peak of tEME is at the same position as the DME peak at the CR (Position A); and iv) the emission peak of ethanol (Position B) is displaced 2″ south-west from the methanol peak.

Concerning the ethyl and propyl species, we note: i) a close correlation between EF and tEME; and ii) ethanol also presents a “V” shape structure (see Fig. 5 of Feng et al. 2015) with the bulk of the emission located away from the CR and coinciding with that of Gt-n-propanol. The ethanol/propanol peak is displaced 1″.5 south from the ethylene glycol $(CH_2OH)_2$ peak (Brouillet et al. 2015), which is a double alcohol and we could naively expect to have the same spatial distribution. Whereas the ethylene glycol peak corresponds to the $^{13}CH_3OH$ peak, the ethanol/propanol peak is the same as that of deuterated methanol (CH_2DOH; see Peng et al. 2012).

Table 1 shows derived column densities and ratios for related species. The derived ratios and the spatial distribution of these molecules suggest important gas phase processes after the evaporation of the mantles of dust grains in hot cores. Possible reactions of the methoxy radical (CH_3O), detected recently in space (Cernicharo et al. 2012), with other species could lead to the increase of chemical complexity in hot cores and hot corinos (Balucani et al. 2015). The spatial stratification of the different species also suggests the time dependent effects on the chemistry of the gas. The detection of the less stable isomers of some species (Tercero et al. 2013) also points in this direction.

To summarize, a combined IRAM 30 m and ALMA SV data study allows us to provide a solid starting point to assess the identification of tEME in the ISM. In addition, some unidentified lines in the source have been assigned to another C_3H_8O isomer, Gt-n-propanol. ALMA maps show different spatial distributions for these species. Whereas tEME seems to mainly arises from the CR component (as well as EF) (Position A), emission from Gt-n-propanol could be located at the south hot core (at the same position as the emission peak of ethanol) (Position B). The CR is no longer the main host of all organic saturated O-bearing species in Orion (see also Peng et al. 2013, for the spatial distribution of acetone and A. López et al., in prep. for the acetic acid emission).

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Appendix A: Online figures and tables

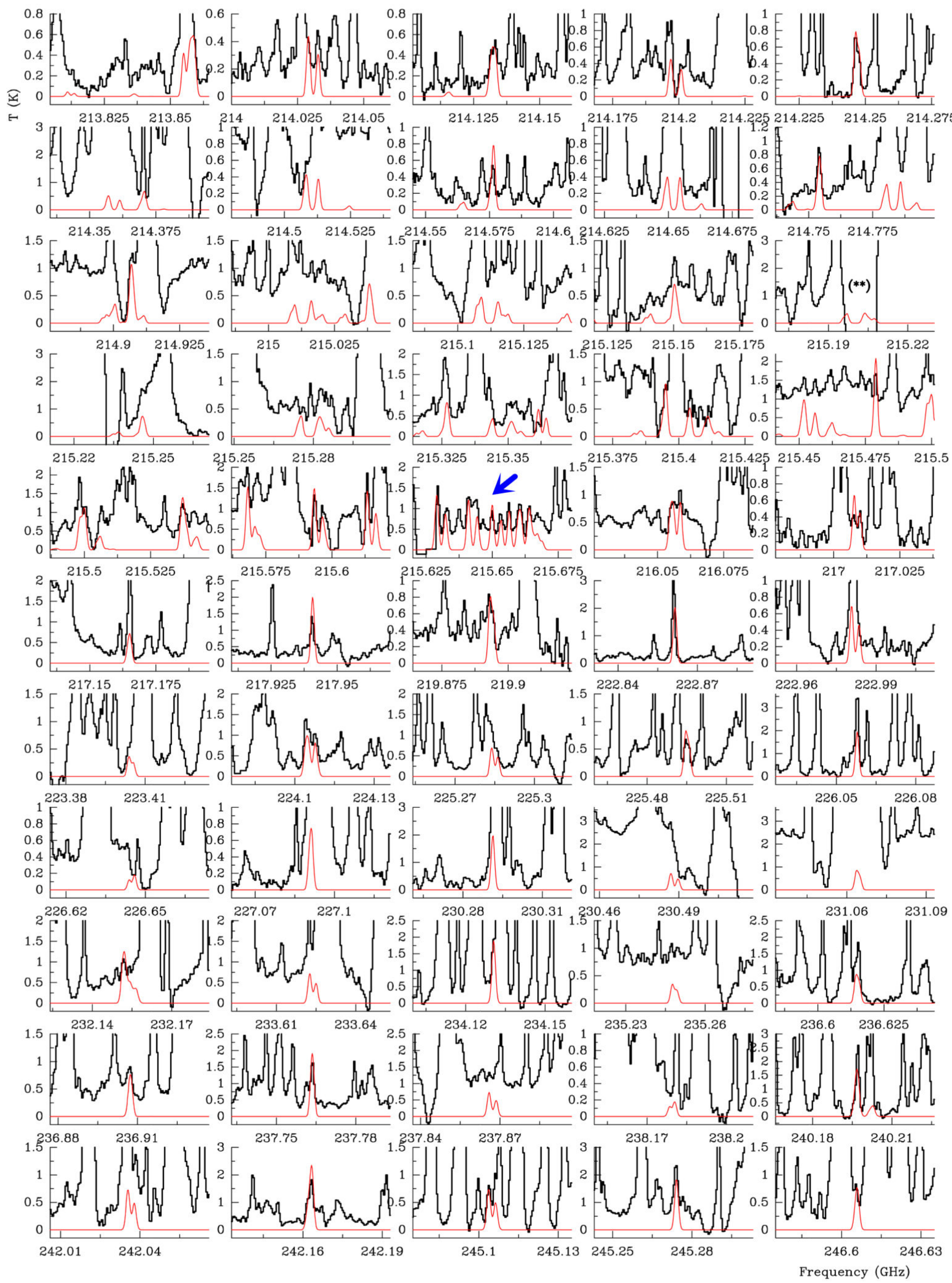

Fig. A.1.

Lines of trans ethyl methyl ether, t-$CH_3CH_2OCH_3$, towards Orion KL detected with the ALMA interferometer in Position A (see text). (**): Features blended with SO (see Table A. 1; artifacts in the spectrum due to the cleaning process). A v_{LSR} of +7.5 km s^{-1} is assumed.

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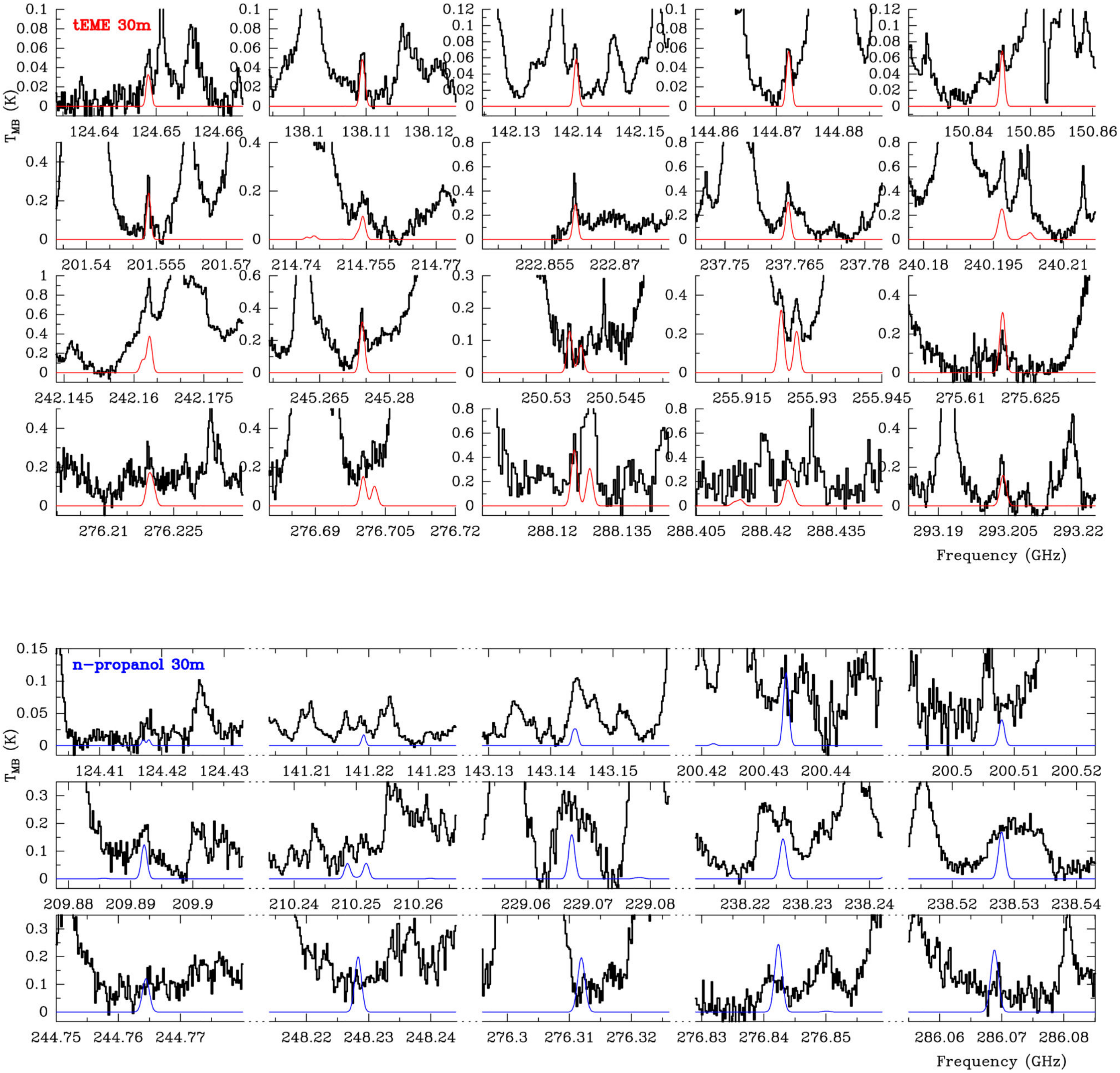

Fig. A.2.

Top panel: selected lines of trans ethyl methyl ether, t-$CH_3CH_2OCH_3$, towards Orion KL detected with the IRAM 30 m telescope. Data in the frequency range 124–151 GHz are those of the survey position. From 201 to 293.5 GHz the data are those of the CR (see Sect. 2), where the emission peak of organic saturated O-rich species such as dimethyl ether (CH_3OCH_3) and methyl formate (CH_3OCOH) is located (Favre et al. 2011; Brouillet et al. 2013). A v_{LSR} of +7.5 km s^{-1} is assumed. *Bottom panel*: selected lines of gauche-trans-n-Propanol, Gt-n-$CH_3CH_2CH_2OH$, towards Orion KL detected with the IRAM 30 m telescope. A v_{LSR} of +7.5 km s^{-1} is assumed.

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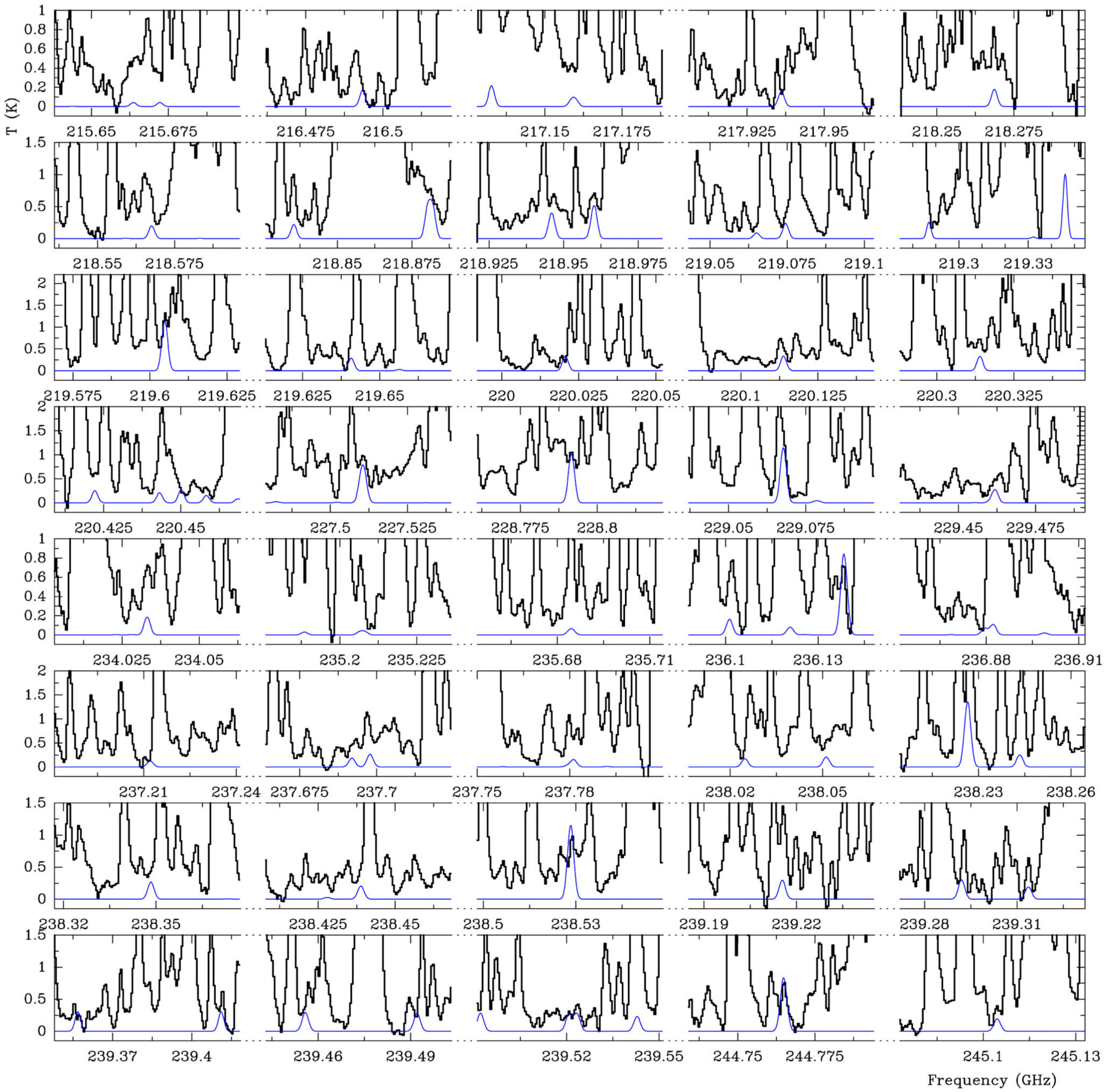

Fig. A.3.

Lines of gauche-trans-n-propanol, Gt-n-$CH_3CH_2CH_2OH$, towards Orion KL detected with the ALMA interferometer in Position B (see text). A v_{LSR} of +8 km s^{-1} is assumed.

Table A.1.

Lines of trans-$CH_3CH_2OCH_3$ in ALMA SV data.

Species	Transition $J_{K_a,K_c} - J'_{K'_a,K'_c}$	Predicted frequency (MHz)	E_{upp} (K)	S_{ij}	Observed frequency (MHz)	*T* (K)	Blends
tEME-EE’	$31_{5,27}$–$31_{4,28}$	213 854.674	220.5	16.34	…	…	CH_3CH_2OH
tEME-EE	$31_{5,27}$–$31_{4,28}$	213 854.982	220.5	16.44	…	…	”
tEME-AE	$31_{5,27}$–$31_{4,28}$	213 855.220	220.5	16.40	…	…	”
tEME-EE	$28_{5,23}$–$28_{4,24}$	213 856.708	185.7	14.17	…	…	”
tEME-AE	$28_{5,23}$–$28_{4,24}$	213 857.473	185.7	13.94	…	…	”
tEME-EE’	$28_{5,23}$–$28_{4,24}$	213 857.509	185.7	13.69	…	…	”
tEME-EA	$31_{5,27}$–$31_{4,28}$	213 858.239	220.5	16.52	…	…	”
tEME-AA	$31_{5,27}$–$31_{4,28}$	213 858.632	220.5	16.53	…	…	”
tEME-EA	$28_{5,23}$–$28_{4,24}$	213 859.015	185.7	14.70	…	…	”
tEME-AA	$28_{5,23}$–$28_{4,24}$	213 859.367	185.7	14.73	…	…	”
tEME-EE’	$30_{5,26}$–$30_{4,27}$	214 028.729	208.6	15.58	…	…	CH_3COCH_3
tEME-EE	$30_{5,26}$–$30_{4,27}$	214 029.157	208.6	15.76	…	…	”
tEME-AE	$30_{5,26}$–$30_{4,27}$	214 029.345	208.6	15.68	…	…	”
tEME-EA	$30_{5,26}$–$30_{4,27}$	214 032.539	208.6	15.91	214 032.3†	0.50	
tEME-AA	$30_{5,26}$–$30_{4,27}$	214 032.539	208.6	15.91	†		
tEME-EE	$27_{5,22}$–$27_{4,23}$	214 131.118	174.9	13.15	214 132.6	0.58	
tEME-AE	$27_{5,22}$–$27_{4,23}$	214 132.010	174.9	12.80	†		
tEME-EE’	$27_{5,22}$–$27_{4,23}$	214 132.166	174.9	12.46	†		
tEME-EA	$27_{5,22}$–$27_{4,23}$	214 133.150	174.9	14.07	†		
tEME-AA	$27_{5,22}$–$27_{4,23}$	214 133.486	174.9	14.14	†		
tEME-EE’	$29_{5,25}$–$29_{4,26}$	214 196.531	196.9	14.73	214 196.8	0.94	
tEME-EE	$29_{5,25}$–$29_{4,26}$	214 197.122	196.9	15.01	†		
tEME-AE	$29_{5,25}$–$29_{4,26}$	214 197.239	196.9	14.88	†		
tEME-EA	$29_{5,25}$–$29_{4,26}$	214 200.673	196.9	15.31	214 201.4	0.41	
tEME-AA	$29_{5,25}$–$29_{4,26}$	214 201.091	196.9	15.31	†		
tEME-EE’	$21_{2,20}$–$20_{1,19}$	214 246.202	93.7	7.76	214 246.5	0.72	
tEME-EE	$21_{2,20}$–$20_{1,19}$	214 246.202	93.7	7.76	†		
tEME-AE	$21_{2,20}$–$20_{1,19}$	214 246.332	93.7	7.76	†		
tEME-EA	$21_{2,20}$–$20_{1,19}$	214 247.602	93.7	7.76	†		
tEME-AA	$21_{2,20}$–$20_{1,19}$	214 247.732	93.7	7.76	†		
tEME-EE’	$26_{5,22}$–$26_{4,22}$	214 355.828	164.4	2.47	…	…	CH_3CH_2OH; SO
tEME-EE’	$28_{5,24}$–$28_{4,25}$	214 356.510	185.7	13.69	…	…	”
tEME-AE	$26_{5,22}$–$26_{4,22}$	214 356.963	164.4	2.08	…	…	”
tEME-EE	$26_{5,22}$–$26_{4,22}$	214 357.232	164.4	1.63	…	…	”
tEME-EE	$28_{5,24}$–$28_{4,25}$	214 357.312	185.7	14.17	…	…	”
tEME-AE	$28_{5,24}$–$28_{4,25}$	214 357.333	185.7	13.93	…	…	”
tEME-EA	$28_{5,24}$–$28_{4,25}$	214 361.091	185.7	14.69	…	…	CH_3OCH_3

Species	Transition $J_{K_a,K_c} - J'_{K'_a,K'_c}$	Predicted frequency (MHz)	E_{upp} (K)	S_{ij}	Observed frequency (MHz)	T (K)	Blends
tEME-AA	$28_{5,24}–28_{4,25}$	214 361.527	185.7	14.72	…	…	”
tEME-EE	$26_{5,21}–26_{4,22}$	214 369.161	164.4	11.92	…	…	CH_3COOCH_3
tEME-AE	$26_{5,21}–26_{4,22}$	214 370.185	164.4	11.47	…	…	”
tEME-EE’	$26_{5,21}–26_{4,22}$	214 370.456	164.4	11.08	…	…	”
tEME-EA	$26_{5,21}–26_{4,22}$	214 370.843	164.4	13.42	…	…	”
tEME-AA	$26_{5,21}–26_{4,22}$	214 371.154	164.4	13.55	…	…	”
tEME-EE’	$27_{5,23}–27_{4,24}$	214 507.462	174.9	12.45	214 508.5	0.61	
tEME-AE	$27_{5,23}–27_{4,24}$	214 508.414	174.9	12.79	†		
tEME-EE	$27_{5,23}–27_{4,24}$	214 508.510	174.9	13.14	†		
tEME-EA	$27_{5,23}–27_{4,24}$	214 512.591	174.9	14.06	…	…	CH_3OCOH $v_t = 1$
tEME-AA	$27_{5,23}–27_{4,24}$	214 513.051	174.9	14.13	…	…	”
tEME-EE	$25_{5,20}–25_{4,21}$	214 575.213	154.4	10.56	214 576.5	0.58	
tEME-AE	$25_{5,20}–25_{4,21}$	214 576.349	154.4	10.10	†		
tEME-EA	$25_{5,20}–25_{4,21}$	214 576.498	154.4	12.69	†		
tEME-EE’	$25_{5,20}–25_{4,21}$	214 576.706	154.4	9.74	†		
tEME-AA	$25_{5,20}–25_{4,21}$	214 576.769	154.4	12.96	†		
tEME-EE’	$26_{5,22}–26_{4,23}$	214 648.535	164.4	11.08	…	…	CH_3OCOH
tEME-AE	$26_{5,22}–26_{4,23}$	214 649.611	164.4	11.47	…	…	”
tEME-EE	$26_{5,22}–26_{4,23}$	214 649.829	164.4	11.92	…	…	”
tEME-EA	$26_{5,22}–26_{4,23}$	214 654.288	164.5	13.41	…	…	”
tEME-AA	$26_{5,22}–26_{4,23}$	214 654.781	164.5	13.54	…	…	”
tEME-EE	$24_{5,19}–24_{4,20}$	214 753.118	144.7	9.23	214 754.0	0.94	
tEME-EA	$24_{5,19}–24_{4,20}$	214 754.023	144.7	11.84	†		
tEME-AA	$24_{5,19}–24_{4,20}$	214 754.233	144.7	12.38	†		
tEME-AE	$24_{5,19}–24_{4,20}$	214 754.329	144.7	8.86	†		
tEME-EE’	$24_{5,19}–24_{4,20}$	214 754.733	144.7	8.60	†		
tEME-EE’	$25_{5,21}–25_{4,22}$	214 779.208	154.4	9.73	…	…	CH_3OCOH
tEME-AE	$25_{5,21}–25_{4,22}$	214 780.378	154.4	10.10	…	…	”
tEME-EE	$25_{5,21}–25_{4,22}$	214 780.701	154.4	10.56	…	…	”
tEME-EA	$25_{5,21}–25_{4,22}$	214 785.581	154.4	12.69	…	…	”
tEME-AA	$25_{5,21}–25_{4,22}$	214 786.123	154.4	12.96	…	…	”
tEME-EE’	$23_{5,19}–23_{4,19}$	214 895.777	135.4	4.03	…	…	CH_3OCOH $v_t = 1$
tEME-AE	$23_{5,19}–23_{4,19}$	214 897.184	135.4	3.90	…	…	”
tEME-EE	$23_{5,19}–23_{4,19}$	214 897.739	135.4	3.67	…	…	”
tEME-EE’	$24_{5,20}–24_{4,21}$	214 899.228	144.7	8.61	…	…	”
tEME-AE	$24_{5,20}–24_{4,21}$	214 900.454	144.7	8.87	…	…	”
tEME-EE	$24_{5,20}–24_{4,21}$	214 900.844	144.7	9.23	…	…	”
tEME-EA	$23_{5,19}–23_{4,19}$	214 903.639	144.7	1.05	…	…	”
tEME-EA	$24_{5,20}–24_{4,21}$	214 906.128	144.7	11.83	214 906.7	1.30	
tEME-EE	$23_{5,18}–23_{4,19}$	214 906.260	135.4	8.13	†		

Species	Transition $J_{K_a,K_c} - J'_{K'_a,K'_c}$	Predicted frequency (MHz)	E_{upp} (K)	S_{ij}	Observed frequency (MHz)	T (K)	Blends
tEME-AA	$24_{5,20}–24_{4,21}$	214 906.739	144.7	12.38	†		
tEME-EA	$23_{5,18}–23_{4,19}$	214 906.872	135.4	10.76	†		
tEME-AA	$23_{5,18}–23_{4,19}$	214 906.992	135.4	11.80	†		
tEME-AE	$23_{5,18}–23_{4,19}$	214 907.507	135.4	7.91	†		
tEME-EE'	$23_{5,18}–23_{4,19}$	214 907.507	135.4	7.77	†		
tEME-EE	$24_{5,19}–24_{4,21}$	214 909.858	144.7	11.83	…	…	CH_3CH_2CN
tEME-EA	$24_{5,19}–24_{4,21}$	214 910.548	144.7	0.55	…	…	”
tEME-AE	$24_{5,19}–24_{4,21}$	214 911.166	144.7	3.51	…	…	”
tEME-EE'	$24_{5,19}–24_{4,21}$	214 911.685	144.7	3.77	…	…	”
tEME-EE'	$23_{5,19}–23_{4,20}$	215 008.545	135.4	7.77	…	…	CH_3OCOH $v_t = 2$
tEME-AE	$23_{5,19}–23_{4,20}$	215 009.791	135.4	7.91	…	…	”
tEME-EE	$23_{5,19}–23_{4,20}$	215 010.209	135.4	8.13	…	…	”
tEME-EA	$23_{5,19}–23_{4,20}$	215 015.810	135.4	10.75	215 016.5	1.16	
tEME-AA	$23_{5,19}–23_{4,20}$	215 016.519	135.4	11.80	†		
tEME-EE	$23_{5,18}–23_{4,20}$	215 018.730	135.4	3.67	…	…	CH_3OCOD
tEME-EA	$23_{5,18}–23_{4,20}$	215 019.043	135.4	1.05	…	…	”
tEME-AE	$23_{5,18}–23_{4,20}$	215 020.114	135.4	3.90	…	…	”
tEME-EE'	$23_{5,18}–23_{4,20}$	215 020.693	135.4	4.03	…	…	”
tEME-EE'	$22_{5,18}–22_{4,18}$	215 027.250	126.6	4.02	…	…	U-line
tEME-AE	$22_{5,18}–22_{4,18}$	215 028.719	126.6	3.99	…	…	”
tEME-EE	$22_{5,18}–22_{4,18}$	215 029.330	126.6	4.00	…	…	”
tEME-EA	$22_{5,18}–22_{4,18}$	215 035.544	126.6	1.78	…	…	CH_3OCOD,CH_3COOCH_3
tEME-EE	$22_{5,17}–22_{4,18}$	215 037.639	126.6	7.33	…	…	”
tEME-EA	$22_{5,17}–22_{4,18}$	215 038.085	126.6	9.45	…	…	”
tEME-AA	$22_{5,17}–22_{4,18}$	215 038.089	126.6	11.23	…	…	CH_3CH_2CN
tEME-AE	$22_{5,17}–22_{4,18}$	215 038.890	126.6	7.24	…	…	”
tEME-EE'	$22_{5,17}–22_{4,18}$	215 039.292	126.6	7.21	…	…	”
tEME-AA	$35_{2,33}–34_{3,32}$	215 107.148	250.8	9.27	…	…	CH_3COOCH_3, CH_3OCOH $v_t = 2$
tEME-EA	$35_{2,33}–34_{3,32}$	215 107.270	250.8	9.27	…	…	”
tEME-EE'	$22_{5,18}–22_{4,19}$	215 107.270	126.6	7.21	…	…	”
tEME-AE	$22_{5,18}–22_{4,19}$	215 108.508	126.6	7.24	…	…	”
tEME-EE	$22_{5,18}–22_{4,19}$	215 108.923	126.6	7.33	…	…	”
tEME-AE	$35_{2,33}–34_{3,32}$	215 109.184	250.8	9.27	…	…	”
tEME-EE	$35_{2,33}–34_{3,32}$	215 109.306	250.8	9.27	…	…	”
tEME-EE'	$35_{2,33}–34_{3,32}$	215 109.306	250.8	9.27	…	…	”
tEME-EA	$22_{5,18}–22_{4,19}$	215 114.713	126.6	9.44	…	…	$CH_3O^{13}COH$
tEME-AA	$22_{5,18}–22_{4,19}$	215 115.545	126.6	11.22	…	…	”
tEME-EE	$22_{5,17}–22_{4,19}$	215 117.232	126.6	3.90	…	…	CH_3CH_2CN
tEME-EA	$22_{5,17}–22_{4,19}$	215 117.254	126.6	1.78	…	…	”
tEME-AE	$22_{5,17}–22_{4,19}$	215 118.679	126.6	3.99	…	…	”

Species	Transition $J_{K_a,K_c} - J'_{K'_a,K'_c}$	Predicted frequency (MHz)	E_{upp} (K)	S_{ij}	Observed frequency (MHz)	*T* (K)	Blends
tEME-EE’	$22_{5,17}$–$22_{4,19}$	215 119.312	126.6	4.02	…	…	”
tEME-EE’	$21_{5,17}$–$21_{4,17}$	215 139.474	118.0	3.75	…	…	$CH_3O^{13}COH$ $v_t = 1$
tEME-AE	$21_{5,17}$–$21_{4,17}$	215 141.013	118.0	3.82	215 141.0	0.59	$CH_3O^{13}COH$ $v_t = 1$
tEME-EE	$21_{5,17}$–$21_{4,17}$	215 141.682	118.0	3.85	†		
tEME-EA	$21_{5,17}$–$21_{4,17}$	215 148.139	118.0	2.58	215 150.7	1.28	
tEME-EE	$21_{5,16}$–$21_{4,17}$	215 149.914	118.0	6.81	†		
tEME-AA	$21_{5,16}$–$21_{4,17}$	215 150.202	118.0	10.66	†		
tEME-EA	$21_{5,16}$–$21_{4,17}$	215 150.327	118.0	8.07	†		
tEME-AE	$21_{5,16}$–$21_{4,17}$	215 151.142	118.0	6.84	215 150.7†	1.28	
tEME-EE’	$21_{5,16}$–$21_{4,17}$	215 151.503	118.0	6.91	†		
tEME-EE’	$22_{5,17}$–$22_{4,18}$	215 195.665	118.0	6.91	…	…	SO
tEME-AE	$22_{5,17}$–$22_{4,18}$	215 196.869	118.0	6.84	…	…	”
tEME-EE	$22_{5,17}$–$22_{4,18}$	215 197.254	118.0	6.81	…	…	”
tEME-EA	$22_{5,17}$–$22_{4,18}$	215 203.100	118.0	8.07	…	…	”
tEME-AA	$22_{5,17}$–$22_{4,18}$	215 204.068	118.0	10.66	…	…	”
tEME-EA	$22_{5,16}$–$22_{4,18}$	215 205.287	118.0	2.58	…	…	”
tEME-EE	$22_{5,16}$–$22_{4,18}$	215 205.486	118.0	3.84	…	…	”
tEME-AE	$22_{5,16}$–$22_{4,18}$	215 206.998	118.0	3.82	…	…	”
tEME-EE’	$22_{5,16}$–$22_{4,18}$	215 207.694	118.0	3.75	…	…	”
tEME-EE’	$20_{5,16}$–$20_{4,16}$	215 234.851	109.9	3.26	…	…	”
tEME-AE	$20_{5,16}$–$20_{4,16}$	215 236.480	109.9	3.41	…	…	”
tEME-EE	$20_{5,16}$–$20_{4,16}$	215 237.223	109.9	3.55	…	…	”
tEME-EA	$20_{5,16}$–$20_{4,16}$	215 243.901	109.9	3.19	…	…	CH_3COOCH_3 $CH_3O^{13}COH$, CH_3CH_2CN v_{13}/v_{21}
tEME-EE	$20_{5,15}$–$20_{4,16}$	215 245.438	109.9	6.54	…	…	”
tEME-AA	$20_{5,15}$–$20_{4,16}$	215 245.691	109.9	10.09	…	…	”
tEME-EA	$20_{5,15}$–$20_{4,16}$	215 245.934	109.9	6.89	…	…	”
tEME-AE	$20_{5,15}$–$20_{4,16}$	215 246.615	109.9	6.67	…	…	”
tEME-EE’	$20_{5,15}$–$20_{4,16}$	215 246.907	109.9	6.83	…	…	”
tEME-EE’	$20_{5,16}$–$20_{4,17}$	215 274.126	109.9	6.83	…	…	CH_3COOCH_3, U-line
tEME-AE	$20_{5,16}$–$20_{4,17}$	215 275.268	109.9	6.67	…	…	”
tEME-EE	$20_{5,16}$–$20_{4,17}$	215 275.595	109.9	6.54	…	…	”
tEME-EA	$20_{5,16}$–$20_{4,17}$	215 281.378	109.9	6.89	…	…	U-line
tEME-AA	$20_{5,16}$–$20_{4,17}$	215 282.470	109.9	10.09	…	…	”
tEME-EA	$20_{5,15}$–$20_{4,17}$	215 283.411	109.9	3.19	…	…	”
tEME-EE	$20_{5,15}$–$20_{4,17}$	215 283.810	109.9	3.55	…	…	”
tEME-AE	$20_{5,15}$–$20_{4,17}$	215 285.403	109.9	3.41	…	…	”
tEME-EE’	$20_{5,15}$–$20_{4,17}$	215 286.182	109.9	3.26	…	…	”
tEME-EE’	$19_{5,15}$–$19_{4,15}$	215 315.464	102.2	2.57	…	…	U-line
tEME-AE	$19_{5,15}$–$19_{4,15}$	215 317.213	102.2	2.79	215 317.4	0.54	U-line

Species	Transition $J_{K_a,K_c} - J'_{K'_a,K'_c}$	Predicted frequency (MHz)	E_{upp} (K)	S_{ij}	Observed frequency (MHz)	*T* (K)	Blends
tEME-EE	$19_{5,15}$–$19_{4,15}$	215 318.057	102.2	3.02	†		
tEME-EA	$19_{5,15}$–$19_{4,15}$	215 324.992	102.2	3.49	215 327.2	1.96	$^{13}CH_3OCOH$ $v_t = 1$
tEME-EE	$19_{5,14}$–$19_{4,15}$	215 326.280	102.2	6.50	†		
tEME-AA	$19_{5,14}$–$19_{4,15}$	215 326.637	102.2	9.52	†		
tEME-EA	$19_{5,14}$–$19_{4,15}$	215 326.971	102.2	6.03	†		
tEME-AE	$19_{5,14}$–$19_{4,15}$	215 327.373	102.2	6.72	†		
tEME-EE’	$19_{5,14}$–$19_{4,15}$	215 327.561	102.2	6.95	†		
tEME-EE’	$19_{5,15}$–$19_{4,16}$	215 343.169	102.2	6.95	…	…	CH_3OCOH
tEME-AE	$19_{5,15}$–$19_{4,16}$	215 344.214	102.2	6.72	…	…	”
tEME-EE	$19_{5,15}$–$19_{4,16}$	215 344.450	102.2	6.50	…	…	”
tEME-EA	$19_{5,15}$–$19_{4,16}$	215 350.059	102.2	6.03	215 351.2	0.91	CH_3CH_2CN ($v = 0$, v_{13}/v_{21})
tEME-AA	$19_{5,15}$–$19_{4,16}$	215 351.248	102.2	9.52	†		
tEME-EA	$19_{5,14}$–$19_{4,16}$	215 352.037	102.2	3.49	†		
tEME-EE	$19_{5,14}$–$19_{4,16}$	215 352.674	102.2	3.02	†		
tEME-AE	$19_{5,14}$–$19_{4,16}$	215 354.374	102.2	2.79	…	…	CH_3CH_2CN ($v = 0$, v_{13}/v_{21})
tEME-EE’	$19_{5,14}$–$19_{4,16}$	215 355.266	102.2	2.57	…	…	”
tEME-EE’	$12_{3,10}$–$11_{2,9}$	215 361.252	40.5	4.16	215 361.7	0.43	
tEME-EE	$12_{3,10}$–$11_{2,9}$	215 361.484	40.5	4.18	†		
tEME-AE	$12_{3,10}$–$11_{2,9}$	215 361.676	40.5	4.17	†		
tEME-EA	$12_{3,10}$–$11_{2,9}$	215 364.224	40.5	4.19	…	…	CH_3CH_2OH
tEME-AA	$12_{3,10}$–$11_{2,9}$	215 364.533	40.5	4.20	…	…	”
tEME-EA	$18_{5,14}$–$18_{4,14}$	215 393.299	94.8	3.48	215 395.5	1.01	
tEME-EE	$18_{5,13}$–$18_{4,14}$	215 394.256	94.8	6.65	†		
tEME-AA	$18_{5,13}$–$18_{4,14}$	215 394.875	94.8	8.95	†		
tEME-AE	$18_{5,13}$–$18_{4,14}$	215 395.227	94.8	6.94	†		
tEME-EA	$18_{5,13}$–$18_{4,14}$	215 395.264	94.8	5.47	†		
tEME-EE’	$18_{5,13}$–$18_{4,14}$	215 395.280	94.8	7.19	†		
tEME-EE’	$18_{5,14}$–$18_{4,15}$	215 403.394	94.8	7.19	215 404.5	0.91	
tEME-AE	$18_{5,14}$–$18_{4,15}$	215 404.308	94.8	6.94	†		
tEME-EE	$18_{5,14}$–$18_{4,15}$	215 404.417	94.8	6.65	†		
tEME-EA	$18_{5,14}$–$18_{4,15}$	215 409.728	94.8	5.47	215 411.2	0.59	
tEME-AA	$18_{5,14}$–$18_{4,15}$	215 410.979	94.8	8.95	†		
tEME-EA	$18_{5,14}$–$18_{4,15}$	215 411.693	94.8	3.48	†		
tEME-EE	$18_{5,14}$–$18_{4,15}$	215 412.657	94.8	2.31	†		
tEME-EA	$17_{5,13}$–$17_{4,13}$	215 450.467	87.9	3.22	215 451.7	1.65	
tEME-EE	$17_{5,12}$–$17_{4,13}$	215 450.974	87.9	6.90	†		
tEME-EE’	$17_{5,12}$–$17_{4,13}$	215 451.703	87.9	7.39	†		
tEME-AE	$17_{5,12}$–$17_{4,13}$	215 451.799	87.9	7.18	†		
tEME-AA	$17_{5,12}$–$17_{4,13}$	215 452.025	87.9	8.39	†		

Species	Transition $J_{K_a,K_c} - J'_{K'_a,K'_c}$	Predicted frequency (MHz)	E_{upp} (K)	S_{ij}	Observed frequency (MHz)	T (K)	Blends
tEME-EA	$17_{5,12}$–$17_{4,13}$	215 452.436	87.9	5.17	†		
tEME-EE’	$17_{5,13}$–$17_{4,13}$	215 455.422	87.9	7.39	215 456.2	1.60	$^{13}CH_3OCOH$ $v_t = 1$
tEME-EE	$17_{5,13}$–$17_{4,13}$	215 456.151	87.9	6.90	†		
tEME-AE	$17_{5,13}$–$17_{4,13}$	215 456.193	87.9	7.18	†		
tEME-EA	$17_{5,13}$–$17_{4,14}$	215 461.025	87.9	5.17	215 462.2	1.81	U-line
tEME-AA	$17_{5,13}$–$17_{4,14}$	215 462.304	87.9	8.39	†		
tEME-EA	$17_{5,12}$–$17_{4,14}$	215 462.994	87.9	3.22	†		
tEME-EE’	$27_{1,27}$–$26_{0,26}$	215 478.840	144.2	21.60	215 479.5	1.81	
tEME-EE	$27_{1,27}$–$26_{0,26}$	215 478.840	144.2	21.60	†		
tEME-AE	$27_{1,27}$–$26_{0,26}$	215 478.854	144.2	21.60	†		
tEME-EA	$27_{1,27}$–$26_{0,26}$	215 479.025	144.2	21.60	†		
tEME-AA	$27_{1,27}$–$26_{0,26}$	215 479.039	144.2	21.60	†		
tEME-EE	$16_{5,11}$–$16_{4,12}$	215 497.897	81.3	7.05	215 498.7	1.96	CH_3CH_2CN v_{13}/v_{21}
tEME-EA	$16_{5,12}$–$16_{4,12}$	215 497.943	81.3	2.74	†		
tEME-EE’	$16_{5,11}$–$16_{4,12}$	215 498.372	81.3	7.37	†		
tEME-AE	$16_{5,11}$–$16_{4,12}$	215 498.590	81.3	7.23	†		
tEME-AA	$16_{5,11}$–$16_{4,12}$	215 499.524	81.3	7.82	215 500.2†	1.22	
tEME-EE’	$16_{5,12}$–$16_{4,13}$	215 499.830	81.3	7.37	†		
tEME-EA	$16_{5,11}$–$16_{4,12}$	215 499.921	81.3	5.08	†		
tEME-EE	$16_{5,12}$–$16_{4,13}$	215 500.305	81.3	7.05	†		
tEME-AE	$16_{5,12}$–$16_{4,13}$	215 500.485	81.3	7.24	†		
tEME-EA	$16_{5,12}$–$16_{4,13}$	215 504.636	81.3	5.08	215 506.2	1.22	$CH_3C^{13}CH$
tEME-AA	$16_{5,12}$–$16_{4,13}$	215 505.905	81.3	7.82	†		
tEME-EA	$16_{5,11}$–$16_{4,13}$	215 506.613	81.3	2.74	†		
tEME-EE	$15_{5,10}$–$15_{4,11}$	215 536.404	75.1	6.94	215 537.7	1.33	
tEME-EE’	$15_{5,10}$–$15_{4,11}$	215 536.720	75.1	7.08	†		
tEME-EA	$15_{5,11}$–$15_{4,11}$	215 537.002	75.1	2.05	†		
tEME-AE	$15_{5,10}$–$15_{4,11}$	215 537.010	75.1	7.03	†		
tEME-EE’	$15_{5,11}$–$15_{4,12}$	215 537.169	75.1	7.08	†		
tEME-EE	$15_{5,11}$–$15_{4,12}$	215 537.485	75.1	6.94	†		
tEME-AE	$15_{5,11}$–$15_{4,12}$	215 537.757	75.1	7.08	†		
tEME-AA	$15_{5,10}$–$15_{4,11}$	215 538.650	75.1	7.25	†		
tEME-EA	$15_{5,10}$–$15_{4,11}$	215 538.990	75.1	5.21	†		
tEME-EA	$15_{5,11}$–$15_{4,12}$	215 541.270	75.1	5.21	215 541.5†	1.06	CH_3COOCH_3
tEME-AA	$15_{5,11}$–$15_{4,12}$	215 542.488	75.1	7.25	†		
tEME-EA	$15_{5,10}$–$15_{4,12}$	215 543.258	75.1	2.05	…		
tEME-EE	$14_{5,9}$–$14_{4,10}$	215 567.750	69.3	6.58	215 567.9	2.13	
tEME-EE’	$14_{5,9}$–$14_{4,10}$	215 567.993	69.3	6.63	†		
tEME-EE’	$14_{5,10}$–$14_{4,11}$	215 568.043	69.3	6.63	†		
tEME-EE	$14_{5,10}$–$14_{4,11}$	215 568.286	69.3	6.58	†		

Species	Transition $J_{K_a,K_c} - J'_{K'_a,K'_c}$	Predicted frequency (MHz)	E_{upp} (K)	S_{ij}	Observed frequency (MHz)	T (K)	Blends
tEME-AE	$14_{5,9}$–$14_{4,10}$	215 568.316	69.3	6.61	†		
tEME-AE	$14_{5,10}$–$14_{4,11}$	215 568.602	69.3	6.61	215 571.7	1.89	CH_3OCOH $v_t = 1$
tEME-AE	$14_{5,10}$–$14_{4,10}$	215 568.774	69.3	1.23	†		
tEME-AA	$14_{5,9}$–$14_{4,10}$	215 570.539	69.3	6.68	†		
tEME-EA	$14_{5,9}$–$14_{4,10}$	215 570.772	69.3	5.45	†		
tEME-EA	$14_{5,10}$–$14_{4,11}$	215 571.650	69.3	5.45	†		
tEME-AA	$14_{5,10}$–$14_{4,11}$	215 572.766	69.3	6.68	†		
tEME-EA	$14_{5,9}$–$14_{4,11}$	215 573.648	69.3	1.23	†		
tEME-EE	$13_{5,8}$–$13_{4,9}$	215 593.014	63.9	6.08	215 593.5	1.41	
tEME-EE’	$13_{5,9}$–$13_{4,10}$	215 593.138	63.9	6.09	†		
tEME-EE’	$13_{5,8}$–$13_{4,9}$	215 593.228	63.9	6.09	†		
tEME-EE	$13_{5,9}$–$13_{4,10}$	215 593.353	63.9	6.08	†		
tEME-AE	$13_{5,8}$–$13_{4,9}$	215 593.566	63.9	6.09	†		
tEME-AE	$13_{5,9}$–$13_{4,10}$	215 593.687	63.9	6.09	†		
tEME-EA	$13_{5,9}$–$13_{4,9}$	215 594.282	63.9	0.53	†		
tEME-AA	$13_{5,8}$–$13_{4,9}$	215 596.207	63.9	6.11	215 596.5	1.12	
tEME-EA	$13_{5,8}$–$13_{4,9}$	215 596.289	63.9	5.58	†		
tEME-EA	$13_{5,9}$–$13_{4,10}$	215 596.478	63.9	5.58	†		
tEME-AA	$13_{5,9}$–$13_{4,10}$	215 597.447	63.9	6.11	†		
tEME-EA	$13_{5,8}$–$13_{4,10}$	215 598.486	63.9	0.53	†		
tEME-EE	$12_{5,7}$–$12_{4,8}$	215 613.102	58.9	5.52	215 613.7	1.89	
tEME-EE’	$12_{5,8}$–$12_{4,9}$	215 613.172	58.9	5.53	†		
tEME-EE’	$12_{5,7}$–$12_{4,8}$	215 613.308	58.9	5.53	†		
tEME-EE	$12_{5,8}$–$12_{4,9}$	215 613.378	58.9	5.52	†		
tEME-AE	$12_{5,7}$–$12_{4,8}$	215 613.651	58.9	5.52	†		
tEME-AE	$12_{5,8}$–$12_{4,9}$	215 613.720	58.9	5.52	†		
tEME-EA	$12_{5,8}$–$12_{4,9}$	215 616.405	58.9	5.37	…	…	$^{13}CH_3OCOH$ $v_t = 1$, CH_3CH_2CN
tEME-EA	$12_{5,7}$–$12_{4,8}$	215 616.490	58.9	5.37	…	…	”
tEME-AA	$12_{5,7}$–$12_{4,8}$	215 616.564	58.9	5.53	…	…	”
tEME-AA	$12_{5,8}$–$12_{4,9}$	215 617.221	58.9	5.53	…	…	”
tEME-EE	$11_{5,6}$–$11_{4,7}$	215 628.800	54.3	4.94	215 629.7	1.60	
tEME-EE’	$11_{5,7}$–$11_{4,8}$	215 628.855	54.3	4.94	†		
tEME-EE’	$11_{5,6}$–$11_{4,7}$	215 629.003	54.3	4.94	†		
tEME-EE	$11_{5,7}$–$11_{4,8}$	215 629.058	54.3	4.94	†		
tEME-AE	$11_{5,6}$–$11_{4,7}$	215 629.349	54.3	4.94	†		
tEME-AE	$11_{5,7}$–$11_{4,8}$	215 629.404	54.3	4.94	†		
tEME-EA	$11_{5,7}$–$11_{4,8}$	215 632.056	54.3	4.91	215 632.7	1.06	
tEME-EA	$11_{5,6}$–$11_{4,7}$	215 632.229	54.3	4.91	†		
tEME-AA	$11_{5,6}$–$11_{4,7}$	215 632.425	54.3	4.94	†		
tEME-AA	$11_{5,7}$–$11_{4,8}$	215 632.754	54.3	4.94	†		

Species	Transition $J_{K_a,K_c} - J'_{K'_a,K'_c}$	Predicted frequency (MHz)	E_{upp} (K)	S_{ij}	Observed frequency (MHz)	T (K)	Blends
tEME-EE	$10_{5,5}$–$10_{4,6}$	215 640.803	50.0	4.35	215 641.1	1.31	
tEME-EE’	$10_{5,6}$–$10_{4,7}$	215 640.854	50.0	4.35	†		
tEME-EE’	$10_{5,5}$–$10_{4,6}$	215 641.007	50.0	4.35	†		
tEME-EE	$10_{5,6}$–$10_{4,7}$	215 641.058	50.0	4.35	†		
tEME-AE	$10_{5,5}$–$10_{4,6}$	215 641.354	50.0	4.35	†		
tEME-AE	$10_{5,6}$–$10_{4,7}$	215 641.405	50.0	4.35	†		
tEME-EA	$10_{5,6}$–$10_{4,7}$	215 644.051	50.0	4.34	215 644.1	1.26	$^{13}CH_3OCOH$ $v_t = 1$
tEME-EA	$10_{5,5}$–$10_{4,6}$	215 644.248	50.0	4.34	†		
tEME-AA	$10_{5,5}$–$10_{4,6}$	215 644.522	50.0	4.35	†		
tEME-AA	$10_{5,6}$–$10_{4,7}$	215 644.676	50.0	4.35	†		
tEME-EE	$9_{5,4}$–$9_{4,5}$	215 649.740	46.1	3.73	215 650.2	1.02	
tEME-EE’	$9_{5,5}$–$9_{4,6}$	215 649.791	46.1	3.73	†		
tEME-EE’	$9_{5,4}$–$9_{4,5}$	215 649.944	46.1	3.73	†		
tEME-EE	$9_{5,5}$–$9_{4,6}$	215 649.995	46.1	3.73	†		
tEME-AE	$9_{5,4}$–$9_{4,5}$	215 650.292	46.1	3.73	†		
tEME-AE	$9_{5,5}$–$9_{4,6}$	215 650.343	46.1	3.73	†		
tEME-EA	$9_{5,5}$–$9_{4,6}$	215 652.990	46.1	3.73	215 653.2	0.92	
tEME-EA	$9_{5,4}$–$9_{4,5}$	215 653.193	46.1	3.73	†		
tEME-AA	$9_{5,4}$–$9_{4,5}$	215 653.509	46.1	3.73	†		
tEME-AA	$9_{5,5}$–$9_{4,6}$	215 653.575	46.1	3.73	†		
tEME-EE	$8_{5,3}$–$8_{4,4}$	215 656.176	42.7	3.10	215 656.2	1.16	
tEME-EE’	$8_{5,4}$–$8_{4,5}$	215 656.227	42.7	3.10	†		
tEME-EE’	$8_{5,3}$–$8_{4,4}$	215 656.380	42.7	3.10	†		
tEME-EE	$8_{5,4}$–$8_{4,5}$	215 656.432	42.7	3.10	†		
tEME-AE	$8_{5,3}$–$8_{4,4}$	215 656.730	42.7	3.10	†		
tEME-AE	$8_{5,4}$–$8_{4,5}$	215 656.781	42.7	3.10	†		
tEME-EA	$8_{5,4}$–$8_{4,5}$	215 659.431	42.7	3.10	215 660.8	1.16	
tEME-EA	$8_{5,3}$–$8_{4,4}$	215 659.635	42.7	3.10	†		
tEME-AA	$8_{5,3}$–$8_{4,4}$	215 659.972	42.7	3.10	†		
tEME-AA	$8_{5,4}$–$8_{4,5}$	215 659.998	42.7	3.10	†		
tEME-EE	$7_{5,2}$–$7_{4,3}$	215 660.620	39.6	2.43	†		
tEME-EE’	$7_{5,3}$–$7_{4,4}$	215 660.672	39.6	2.43	†		
tEME-EE’	$7_{5,2}$–$7_{4,3}$	215 660.825	39.6	2.43	†		
tEME-EE	$7_{5,3}$–$7_{4,4}$	215 660.877	39.6	2.43	†		
tEME-AE	$7_{5,2}$–$7_{4,3}$	215 661.175	39.6	2.43	†		
tEME-AE	$7_{5,3}$–$7_{4,4}$	215 661.227	39.6	2.43	†		
tEME-EE	$6_{5,1}$–$6_{4,2}$	215 663.523	36.9	1.72	215 664.6	1.11	
tEME-EE’	$6_{5,2}$–$6_{4,3}$	215 663.575	36.9	1.72	†		
tEME-EE’	$6_{5,1}$–$6_{4,2}$	215 663.728	36.9	1.72	†		
tEME-EE	$6_{5,2}$–$6_{4,3}$	215 663.780	36.9	1.72	†		

Species	Transition $J_{K_a,K_c} - J'_{K'_a,K'_c}$	Predicted frequency (MHz)	E_{upp} (K)	S_{ij}	Observed frequency (MHz)	*T* (K)	Blends
tEME-EA	$7_{5,3}$–$7_{4,4}$	215 663.879	39.6	2.43	†		
tEME-AE	$6_{5,1}$–$6_{4,2}$	215 664.080	36.9	1.72	†		
tEME-EA	$7_{5,2}$–$7_{4,3}$	215 664.084	39.6	2.43	†		
tEME-AE	$6_{5,2}$–$6_{4,3}$	215 664.131	36.9	1.72	†		
tEME-AA	$7_{5,2}$–$7_{4,3}$	215 664.430	39.6	2.43	†		
tEME-AA	$7_{5,3}$–$7_{4,4}$	215 664.439	39.6	2.43	†		
tEME-EE	$5_{5,0}$–$5_{4,1}$	215 665.279	34.6	0.92	†		
tEME-EE’	$5_{5,1}$–$5_{4,2}$	215 665.331	34.6	0.92	†		
tEME-EE’	$5_{5,0}$–$5_{4,1}$	215 665.485	34.6	0.92	†		
tEME-EE	$5_{5,1}$–$5_{4,2}$	215 665.537	34.6	0.92	†		
tEME-AE	$5_{5,0}$–$5_{4,1}$	215 665.837	34.6	0.92	†		
tEME-AE	$5_{5,1}$–$5_{4,2}$	215 665.889	34.6	0.92	†		
tEME-EA	$6_{5,2}$–$6_{4,3}$	215 666.786	36.9	1.72	215 667.6	0.97	CH_3CH_2CN
tEME-AE	$6_{5,1}$–$6_{4,2}$	215 666.991	36.9	1.72	†		
tEME-AE	$6_{5,1}$–$6_{4,2}$	215 667.342	36.9	1.72	†		
tEME-EA	$6_{5,2}$–$6_{4,3}$	215 667.344	36.9	1.72	†		
tEME-AE	$5_{5,1}$–$5_{4,2}$	215 668.545	34.6	0.92	†		
tEME-AA	$5_{5,0}$–$5_{4,1}$	215 668.751	34.6	0.92	†		
tEME-AA	$5_{5,0}$–$5_{4,1}$	215 669.103	34.6	0.92	†		
tEME-AE	$5_{5,1}$–$5_{4,2}$	215 669.103	34.6	0.92	†		
tEME-EE’	$6_{4,3}$–$5_{3,3}$	216 054.535	26.5	3.73	216 056.4	0.95	
tEME-EE	$6_{4,3}$–$5_{3,3}$	216 054.868	26.5	3.73	†		
tEME-AE	$6_{4,3}$–$5_{3,3}$	216 055.095	26.5	3.73	†		
tEME-EE	$6_{4,2}$–$5_{3,2}$	216 055.759	26.5	3.73	†		
tEME-EE’	$6_{4,2}$–$5_{3,2}$	216 056.093	26.5	3.73	†		
tEME-AE	$6_{4,2}$–$5_{3,2}$	216 056.319	26.5	3.73	†		
tEME-EA	$6_{4,3}$–$5_{3,3}$	216 058.222	26.5	3.69	216 059.3†	1.14	
tEME-EA	$6_{4,2}$–$5_{3,2}$	216 058.519	26.5	3.69	†		
tEME-AA	$6_{4,3}$–$5_{3,2}$	216 058.597	26.5	3.73	†		
tEME-AA	$6_{4,2}$–$5_{3,3}$	216 058.930	26.5	3.73	†		
tEME-EE	$12_{3,9}$–$11_{2,10}$	217 007.530	40.5	4.14	217 007.6	0.49	
tEME-EE’	$12_{3,9}$–$11_{2,10}$	217 007.763	40.5	4.12	†		
tEME-AE	$12_{3,9}$–$11_{2,10}$	217 007.939	40.5	4.13	†		
tEME-EA	$12_{3,9}$–$11_{2,10}$	217 009.762	40.5	4.16	217 010.6	0.54	
tEME-AA	$12_{3,9}$–$11_{2,10}$	217 010.054	40.5	4.16	†		
tEME-AA	$30_{1,29}$–$29_{2,28}$	217 164.465	182.5	13.55	217 165.1	2.68	CH_3OCOH
tEME-EA	$30_{1,29}$–$29_{2,28}$	217 164.508	182.5	13.55	†		
tEME-AE	$30_{1,29}$–$29_{2,28}$	217 165.360	182.5	13.55	†		
tEME-EE	$30_{1,29}$–$29_{2,28}$	217 165.402	182.5	13.55	†		
tEME-EE’	$30_{1,29}$–$29_{2,28}$	217 165.402	182.5	13.55	†		

Species	Transition $J_{K_a,K_c} - J'_{K'_a,K'_c}$	Predicted frequency (MHz)	E_{upp} (K)	S_{ij}	Observed frequency (MHz)	T (K)	Blends
tEME-AA	$28_{0,28}$–$27_{1,27}$	217 940.650	154.7	22.59	217 940.7	1.46	
tEME-EA	$28_{0,28}$–$27_{1,27}$	217 940.651	154.7	22.59	†		
tEME-AE	$28_{0,28}$–$27_{1,27}$	217 940.758	154.7	22.59	†		
tEME-EE	$28_{0,28}$–$27_{1,27}$	217 940.759	154.7	22.59	†		
tEME-EE’	$28_{0,28}$–$27_{1,27}$	217 940.759	154.7	22.59	†		
tEME-EE’	$22_{2,21}$–$21_{1,20}$	219 893.140	102.2	8.31	219 893.0	0.86	
tEME-EE	$22_{2,21}$–$21_{1,20}$	219 893.140	102.2	8.31	†		
tEME-AE	$22_{2,21}$–$21_{1,20}$	219 893.263	102.2	8.31	†		
tEME-EA	$22_{2,21}$–$21_{1,20}$	219 894.511	102.2	8.31	219 894.5†	0.66	
tEME-AA	$22_{2,21}$–$21_{1,20}$	219 894.635	102.2	8.31	†		
tEME-EE’	$28_{1,28}$–$27_{0,27}$	222 861.487	154.8	22.63	222 861.2	3.06	CH_3OCHO
tEME-EE	$28_{1,28}$–$27_{0,27}$	222 861.487	154.8	22.63	†		
tEME-AE	$28_{1,28}$–$27_{0,27}$	222 861.500	154.8	22.63	†		
tEME-EA	$28_{1,28}$–$27_{0,27}$	222 861.655	154.8	22.63	†		
tEME-AA	$28_{1,28}$–$27_{0,27}$	222 861.668	154.8	22.63	†		
tEME-EE’	$13_{3,11}$–$12_{2,10}$	222 980.574	45.5	4.38	…	…	$CH_3O^{13}COH$
tEME-EE	$13_{3,11}$–$12_{2,10}$	222 980.720	45.5	4.39	…	…	”
tEME-AE	$13_{3,11}$–$12_{2,10}$	222 980.951	45.5	4.39	…	…	”
tEME-EA	$13_{3,11}$–$12_{2,10}$	222 983.368	45.5	4.40	…	…	”
tEME-AA	$13_{3,11}$–$12_{2,10}$	222 983.672	45.5	4.40	…	…	”
tEME-EE	$16_{2,14}$–$15_{1,15}$	223 403.761	57.4	2.48	223 403.5	0.82	CH_3OCH_3
tEME-EE’	$16_{2,14}$–$15_{1,15}$	223 403.762	57.4	2.48	†		
tEME-AE	$16_{2,14}$–$15_{1,15}$	223 404.001	57.4	2.48	†		
tEME-EA	$16_{2,14}$–$15_{1,15}$	223 405.432	57.4	2.48	…	…	CH_3OCH_3
tEME-AA	$16_{2,14}$–$15_{1,15}$	223 405.671	57.4	2.48	…	…	
tEME-EE’	$7_{4,4}$–$6_{3,4}$	224 103.753	29.2	3.89	224 104.2	1.49	
tEME-EE	$7_{4,4}$–$6_{3,4}$	224 104.093	29.2	3.88	†		
tEME-AE	$7_{4,4}$–$6_{3,4}$	224 104.315	29.2	3.89	†		
tEME-EE	$7_{4,3}$–$6_{3,3}$	224 104.926	29.2	3.88	†		
tEME-EE’	$7_{4,3}$–$6_{3,3}$	224 105.266	29.2	3.89	†		
tEME-AE	$7_{4,3}$–$6_{3,3}$	224 105.490	29.2	3.89	†		
tEME-AA	$7_{4,4}$–$6_{3,3}$	224 107.456	29.2	3.90	224 108.0†	1.12	
tEME-EA	$7_{4,4}$–$6_{3,4}$	224 107.546	29.2	3.58	†		
tEME-EA	$7_{4,3}$–$6_{3,3}$	224 107.581	29.2	3.58	†		
tEME-AA	$7_{4,3}$–$6_{3,4}$	224 108.457	29.2	3.90	†		
tEME-EE	$13_{3,10}$–$12_{2,11}$	225 283.674	45.5	4.33	225 283.2	1.41	CH_3CH_2OH
tEME-EE’	$13_{3,10}$–$12_{2,11}$	225 283.820	45.5	4.33	†		
tEME-AE	$13_{3,10}$–$12_{2,11}$	225 284.043	45.5	4.33	†		
tEME-EA	$13_{3,10}$–$12_{2,11}$	225 285.990	45.5	4.34	†		
tEME-AA	$13_{3,10}$–$12_{2,11}$	225 286.286	45.5	4.34	†		

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Species	Transition $J_{K_a,K_c} - J'_{K'_a,K'_c}$	Predicted frequency (MHz)	E_{upp} (K)	S_{ij}	Observed frequency (MHz)	T (K)	Blends
tEME-EE'	$23_{2,22}$–$22_{1,21}$	225 494.508	111.0	8.90	225 494.6	0.72	
tEME-EE	$23_{2,22}$–$22_{1,21}$	225 494.508	111.0	8.90	†		
tEME-AE	$23_{2,22}$–$22_{1,21}$	225 494.625	111.0	8.90	†		
tEME-EA	$23_{2,22}$–$22_{1,21}$	225 495.848	111.0	8.90	†		
tEME-AA	$23_{2,22}$–$22_{1,21}$	225 495.965	111.0	8.90	†		
tEME-EA	$29_{0,29}$–$28_{1,28}$	226 057.836	165.7	23.62	226 058.4	3.50	CH_3CH_2OH
tEME-AA	$29_{0,29}$–$28_{1,28}$	226 057.836	165.7	23.62	†		
tEME-EE	$29_{0,29}$–$28_{1,28}$	226 057.928	165.7	23.62	†		
tEME-EE'	$29_{0,29}$–$28_{1,28}$	226 057.928	165.7	23.62	†		
tEME-AE	$29_{0,29}$–$28_{1,28}$	226 057.928	165.7	23.62	†		
tEME-AA	$31_{1,30}$–$30_{2,29}$	227 090.552	194.5	14.51	…	…	CH_3OH
tEME-EA	$31_{1,30}$–$30_{2,29}$	227 090.589	194.5	14.51	…	…	”
tEME-AE	$31_{1,30}$–$30_{2,29}$	227 091.390	194.5	14.51	…	…	”
tEME-EE	$31_{1,30}$–$30_{2,29}$	227 091.426	194.5	14.51	…	…	”
tEME-EE'	$31_{1,30}$–$30_{2,29}$	227 091.426	194.5	14.51	…	…	”
tEME-EE'	$29_{1,29}$–$28_{0,28}$	230 291.194	165.8	23.66	…	…	CH_3OH, CH_3OCOH
tEME-EE	$29_{1,29}$–$28_{0,28}$	230 291.194	165.8	23.66	…	…	”
tEME-AE	$29_{1,29}$–$28_{0,28}$	230 291.205	165.8	23.66	…	…	”
tEME-EA	$29_{1,29}$–$28_{0,28}$	230 291.345	165.8	23.66	…	…	”
tEME-AA	$29_{1,29}$–$28_{0,28}$	230 291.357	165.8	23.66	…	…	”
tEME-EE'	$14_{3,12}$–$13_{2,11}$	230 486.881	50.9	4.59	230 487.1	0.58	CO
tEME-EE	$14_{3,12}$–$13_{2,11}$	230 486.975	50.9	4.59	†		
tEME-AE	$14_{3,12}$–$13_{2,11}$	230 487.227	50.9	4.59	†		
tEME-EA	$14_{3,12}$–$13_{2,11}$	230 489.569	50.9	4.59	…	…	CO
tEME-AA	$14_{3,12}$–$13_{2,11}$	230 489.869	50.9	4.59	…	…	”
tEME-EE'	$24_{2,23}$–$23_{1,22}$	231 063.540	120.2	9.52	…	…	OCS
tEME-EE	$24_{2,23}$–$23_{1,22}$	231 063.540	120.2	9.52	…	…	”
tEME-AE	$24_{2,23}$–$23_{1,22}$	231 063.652	120.2	9.52	…	…	”
tEME-EA	$24_{2,23}$–$23_{1,22}$	231 064.846	120.2	9.52	…	…	”
tEME-EA	$24_{2,23}$–$23_{1,22}$	231 064.958	120.2	9.52	…	…	”
tEME-EE'	$8_{4,5}$–$7_{3,5}$	232 151.207	32.3	4.03	232 151.8	1.16	
tEME-EE	$8_{4,5}$–$7_{3,5}$	232 151.590	32.3	3.98	†		
tEME-AE	$8_{4,5}$–$7_{3,5}$	232 151.787	32.3	4.01	†		
tEME-EE	$8_{4,4}$–$7_{3,4}$	232 152.098	32.3	3.98	†		
tEME-EE'	$8_{4,4}$–$7_{3,4}$	232 152.480	32.3	4.03	†		
tEME-EA	$8_{4,5}$–$7_{3,4}$	232 152.521	32.3	1.00	†		
tEME-AE	$8_{4,4}$–$7_{3,4}$	232 152.685	32.3	4.01	†		
tEME-AA	$8_{4,5}$–$7_{3,4}$	232 154.033	32.3	4.08	†		
tEME-EA	$8_{4,4}$–$7_{3,4}$	232 154.362	32.3	3.08	†		
tEME-EA	$8_{4,5}$–$7_{3,5}$	232 155.426	32.3	3.08	†		

Species	Transition $J_{K_a,K_c} - J'_{K'_a,K'_c}$	Predicted frequency (MHz)	E_{upp} (K)	S_{ij}	Observed frequency (MHz)	T (K)	Blends
tEME-AA	$8_{4.4}$–$7_{3.5}$	232 156.540	32.3	4.08	…	…	CH_3OCOH v_t = 1
tEME-EA	$8_{4.4}$–$7_{3.5}$	232 157.268	32.3	1.00	…	…	”
tEME-EE	$14_{3,11}$–$13_{2,12}$	233 622.462	51.0	4.51	233 622.5	2.10	CH_3CH_2CN v_{13}/v_{21}
tEME-EE’	$14_{3,11}$–$13_{2,12}$	233 622.556	51.0	4.51	†		
tEME-AE	$14_{3,11}$–$13_{2,12}$	233 622.806	51.0	4.51	†		
tEME-EA	$14_{3.11}$–$13_{2.12}$	233 624.824	51.0	4.51	…	…	CH_3OCOH v_t = 0,1
tEME-AA	$14_{3,11}$–$13_{2,12}$	233 625.121	51.0	4.51	…	…	”
tEME-EA	$30_{0,30}$–$29_{1.29}$	234 130.523	177.0	24.66	…	…	CH_3OCOH
tEME-AA	$30_{0,30}$–$29_{1.29}$	234 130.524	177.0	24.66	…	…	”
tEME-EE	$30_{0,30}$–$29_{1,29}$	234 130.601	177.0	24.66	…	…	”
tEME-EE’	$30_{0,30}$–$29_{1,29}$	234 130.601	177.0	24.66	…	…	”
tEME-AE	$30_{0,30}$–$29_{1,29}$	234 130.602	177.0	24.66	…	…	”
tEME-EE	$17_{2,15}$–$16_{1,16}$	235 247.484	64.0	2.37	235 247.5	0.49	U-line
tEME-EE’	$17_{2,15}$–$16_{1,16}$	235 247.485	64.0	2.37	†		
tEME-AE	$17_{2,15}$–$16_{1,16}$	235 247.731	64.0	2.37	†		
tEME-EA	$17_{2,15}$–$16_{1,16}$	235 249.156	64.0	2.37	235 249.6	0.41	U-line
tEME-AA	$17_{2,15}$–$16_{1,16}$	235 249.403	64.0	2.37	†		
tEME-EE’	$25_{2,24}$–$24_{1,23}$	236 614.358	129.8	10.19	236 614.8	1.89	$CH_3O^{13}COH$ v_t = 1
tEME-EE	$25_{2,24}$–$24_{1,23}$	236 614.358	129.8	10.19	†		
tEME-AE	$25_{2,24}$–$24_{1,23}$	236 614.464	129.8	10.19	†		
tEME-EA	$25_{2,24}$–$24_{1,23}$	236 615.628	129.8	10.19	†		
tEME-AA	$25_{2,24}$–$24_{1,23}$	236 615.733	129.8	10.19	†		
tEME-AA	$32_{1,31}$–$31_{2,30}$	236 906.877	206.9	15.50	236 907.6	0.99	
tEME-EA	$32_{1,31}$–$31_{2,30}$	236 906.908	206.9	15.50	†		
tEME-AE	$32_{1,31}$–$31_{2,30}$	236 907.656	206.9	15.50	†		
tEME-EE	$32_{1,31}$–$31_{2,30}$	236 907.687	206.9	15.50	†		
tEME-EE’	$32_{1,31}$–$31_{2,30}$	236 907.687	206.9	15.50	†		
tEME-EE’	$30_{1,30}$–$29_{0,29}$	237 763.517	177.1	24.69	237 763.2	1.76	
tEME-EE	$30_{1,30}$–$29_{0,29}$	237 763.517	177.1	24.69	†		
tEME-AE	$30_{1,30}$–$29_{0,29}$	237 763.527	177.1	24.69	†		
tEME-EA	$30_{1,30}$–$29_{0,29}$	237 763.653	177.1	24.69	†		
tEME-AA	$30_{1,30}$–$29_{0,29}$	237 763.664	177.1	24.69	†		
tEME-EE’	$15_{3,13}$–$14_{2, 12}$	237 865.715	56.7	4.79	237 866.1	1.40	
tEME-EE	$15_{3,13}$–$14_{2,12}$	237 865.778	56.7	4.80	†		
tEME-AE	$15_{3,13}$–$14_{2,12}$	237 866.042	56.7	4.80	†		
tEME-EA	$15_{3,13}$–$14_{2,12}$	237 868.339	56.7	4.80	…	…	U-line
tEME-AA	$15_{3,13}$–$14_{2,12}$	237 868.635	56.7	4.80	…	…	”
tEME-EA	$9_{4,6}$–$8_{3,5}$	240 195.817	35.8	1.64	240 196.7	2.66	$^{13}CH_3OCOH$
tEME-EE	$9_{4,5}$–$8_{3,5}$	240 196.101	35.8	3.88	†		
tEME-EE’	$9_{4,6}$–$8_{3,6}$	240 196.396	35.8	3.88	†		

Species	Transition $J_{K_a,K_c} - J'_{K'_a,K'_c}$	Predicted frequency (MHz)	E_{upp} (K)	S_{ij}	Observed frequency (MHz)	*T* (K)	Blends
tEME-EE'	$9_{4,5}$–$8_{3,5}$	240 196.642	35.8	3.88	†		
tEME-AE	$9_{4,5}$–$8_{3,5}$	240 196.777	35.8	3.88	†		
tEME-EE	$9_{4,6}$–$8_{3,6}$	240 196.937	35.8	3.88	†		
tEME-AE	$9_{4,6}$–$8_{3,6}$	240 197.045	35.8	3.88	†		
tEME-AA	$9_{4.6}$–$8_{3,5}$	240 197.196	35.8	3.88	†		
tEME-EA	$9_{4,5}$–$8_{3,5}$	240 197.654	35.8	3.88	†		
tEME-EA	$9_{4,6}$–$8_{3,6}$	240 201.478	35.8	2.63	…	…	CH_3OCOH $v_t = 1$
tEME-AA	$9_{4,5}$–$8_{3,6}$	240 202.719	35.8	4.28	…	…	”
tEME-EA	$9_{4,5}$–$8_{3,6}$	240 203.315	35.8	1.64	…	…	”
tEME-EE	$15_{3,12}$–$14_{2,13}$	242 035.318	56.8	4.68	…	…	CH_2DOH; CH_2DCN
tEME-EE'	$15_{3,12}$–$14_{2,13}$	242 035.380	56.8	4.68	…	…	”
tEME-AE	$15_{3,12}$–$14_{2,13}$	242 035.647	56.8	4.68	…	…	”
tEME-EA	$15_{3,12}$–$14_{2,13}$	242 037.704	56.8	4.68	…	…	CH_2DOCOH
tEME-AA	$15_{3,12}$–$14_{2,13}$	242 038.002	56.8	4.68	…	…	”
tEME-EE'	$26_{2,25}$–$25_{1,24}$	242 161.785	139.8	10.89	242 163.3	1.86	
tEME-EE	$26_{2.25}$–$25_{1,24}$	242 161.785	139.8	10.89	†		
tEME-AE	$26_{2,25}$–$25_{1,24}$	242 161.884	139.8	10.89	†		
tEME-EA	$26_{2,25}$–$25_{1,24}$	242 163.015	139.8	10.89	†		
tEME-AA	$26_{2,25}$–$^{25}{}_{1,24}$	242 163.114	139.8	10.89	†		
tEME-EA	$31_{0,31}$–$30_{1,30}$	242 163.369	188.7	25.69	†		
tEME-AA	$31_{0,31}$–$30_{1,30}$	242 163.371	188.7	25.69	†		
tEME-EE	$31_{0,31}$–$30_{1,30}$	242 163.434	188.7	25.69	†		
tEME-EE'	$31_{0,31}$–$30_{1,30}$	242 163.434	188.7	25.69	†		
tEME-AE	$31_{0,31}$–$30_{1,30}$	242 163.436	188.7	25.69	†		
tEME-EE'	$16_{3,14}$–$15_{2,13}$	245 103.550	62.9	4.99	245 103.4	0.92	
tEME-EE	$16_{3,14}$–$15_{2,13}$	245 103.592	62.9	4.99	†		
tEME-AE	$16_{3,14}$–$15_{2,13}$	245 103.864	62.9	4.99	†		
tEME-EA	$16_{3,14}$–$15_{2,13}$	245 106.133	62.9	4.99	245 106.4†	1.13	CH_3OCOH $v_t = 2$
tEME-EA	$16_{3,14}$–$15_{2,13}$	245 106.426	62.9	5.00	†		
tEME-EE'	$31_{1,31}$–$30_{0,30}$	245 274.088	188.8	25.71	245 274.0	2.44	
tEME-EE	$31_{1,31}$–$30_{0,30}$	245 274.088	188.8	25.71	†		
tEME-AE	$31_{1,31}$–$30_{0,30}$	245 274.098	188.8	25.71	†		
tEME-EA	$31_{1,31}$–$30_{0,30}$	245 274.211	188.8	25.71	†		
tEME-AA	$31_{1,31}$–$30_{0,30}$	245 274.221	188.8	25.71	†		
tEME-AA	$33_{1,32}$–$32_{2,31}$	246 605.346	219.6	16.51	246 605.6	0.92	
tEME-EA	$33_{1,32}$–$32_{2,31}$	246 605.372	219.6	16.51	†		
tEME-AE	$33_{1,32}$–$32_{2,31}$	246 606.066	219.6	16.51	†		
tEME-EE	$33_{1,32}$–$32_{2,31}$	246 606.092	219.6	16.51	†		
tEME-EE'	$33_{1,32}$–$32_{2,31}$	246 606.092	219.6	16.51	†		

Notes. Lines of trans-$CH_3CH_2OCH_3$ (tEME) ground state present in the spectral scan of Orion KL from the ALMA interferometer. Column 1 indicates the species, Col. 2 gives the transition, Col. 3 the predicted frequency, Col. 4 upper level energy, Col. 5 the line strength, Col. 6 observed frequency at the peak channel of the line (relative to a v_{LSR} of +7.5 km s^{-1}), Col. 7 brightness temperature at the peak channel of the line, and Col. 8 shows blends with other molecular species.

† Blended with previous line.

Table A.2.

Lines of trans-$CH_3CH_2OCH_3$ in 30 m data.

Species	Transition $J_{K_a,K_c} - J'_{K'_a,K'_c}$	Predicted frequency (MHz)	E_{upp} (K)	S_{ij}	Observed[1] frequency (MHz)	Observed[1] T_{MB} (K)	Model[2] T_{MB} (K)	Blends
tEME-AA	$13_{0,13}$–$12_{1,12}$	88 665.592	35.0	7.66	88 665.8	0.05	0.01	U-line
tEME-EA	$13_{0,13}$–$12_{1,12}$	88 665.628	35.0	7.66	†			
tEME-AE	$13_{0,13}$–$12_{1,12}$	88 666.042	35.0	7.66	†			
tEME-EE	$13_{0,13}$–$12_{1,12}$	88 666.078	35.0	7.66	†			
tEME-EE'	$13_{0,13}$–$12_{1,12}$	88 666.078	35.0	7.66	†			
tEME-EE'	$10_{1,10}$–$9_{0,9}$	97 575.502	22.0	6.04	…	…	0.01	CH_3OH
tEME-EE	$10_{1,10}$–$9_{0,9}$	97 575.502	22.0	6.04	†			
tEME-AE	$10_{1,10}$–$9_{0,9}$	97 575.556	22.0	6.04	†			
tEME-EA	$10_{1,10}$–$9_{0,9}$	97 576.027	22.0	6.04	†			
tEME-AA	$10_{1,10}$–$9_{0,9}$	97 576.081	22.0	6.04	†			
tEME-AA	$14_{0,14}$–$13_{1,13}$	97 678.316	40.4	8.52	…	…	0.01	CH_3OH, CH_3CH_2CN v_{13}/v_{21}
tEME-EA	$14_{0,14}$–$13_{1,13}$	97 678.350	40.4	8.52	†			
tEME-AE	$14_{0,14}$–$13_{1,13}$	97 678.746	40.4	8.52	†			
tEME-EE	$14_{0,14}$–$13_{1,13}$	97 678.779	40.4	8.52	†			
tEME-EE'	$14_{0,14}$–$13_{1,13}$	97 678.779	40.4	8.52	†			
tEME-EE	$26_{3,23}$–$26_{2,24}$	101 017.882	146.4	17.08	…	…	0.01	U-line
tEME-EE'	$26_{3,23}$–$26_{2,24}$	101 017.884	146.4	17.08	†			
tEME-AE	$26_{3,23}$–$26_{2,24}$	101 018.111	146.4	17.08	†			
tEME-EE	$25_{3,22}$–$25_{2,23}$	102 684.892	136.2	16.03	102 684.6	0.07	0.01	^{18}OCS
tEME-EE'	$25_{3,22}$–$25_{2,23}$	102 684.894	136.2	16.03	†			
tEME-AE	$25_{3,22}$–$25_{2,23}$	102 685.127	136.2	16.03	†			
tEME-EE	$24_{3,21}$–$24_{2,22}$	104 364.955	126.5	15.03	…	…	0.01	CH_3CH_2CN
tEME-EE'	$24_{3,21}$–$24_{2,22}$	104 364.959	126.5	15.03	†			
tEME-AE	$24_{3,21}$–$24_{2,22}$	104 365.198	126.5	15.03	†			
tEME-EE'	$11_{1,11}$–$10_{0,10}$	104 401.631	26.2	6.73	…	…	0.02	CH_2CHCN
tEME-EE	$11_{1,11}$–$10_{0,10}$	104 401.631	26.2	6.73	†			
tEME-AE	$11_{1,11}$–$10_{0,10}$	104 401.683	26.2	6.73	†			
tEME-EA	$11_{1,11}$–$10_{0,10}$	104 402.145	26.2	6.73	†			
tEME-AA	$11_{1,11}$–$10_{0,10}$	104 402.196	26.2	6.73	†			
tEME-EE	$23_{3,20}$–$23_{2,21}$	106 030.362	117.2	14.09	…	…	0.01	CH_3OCOH
tEME-EE'	$23_{3,20}$–$23_{2,21}$	106 030.367	117.2	14.09	†			
tEME-AE	$23_{3,20}$–$23_{2,21}$	106 030.611	117.2	14.09	†			
tEME-AA	$15_{0,15}$–$14_{1,14}$	106 666.950	46.1	9.41	…	…	0.02	CH_3OCOH
tEME-EA	$15_{0,15}$–$14_{1,14}$	106 666.980	46.1	9.41	†			
tEME-AE	$15_{0,15}$–$14_{1,14}$	106 667.358	46.1	9.41	†			
tEME-EE	$15_{0,15}$–$14_{1,14}$	106 667.388	46.1	9.41	†			

Species	Transition $J_{K_a,K_c} - J'_{K'_a,K'_c}$	Predicted frequency (MHz)	E_{upp} (K)	S_{ij}	Observed[1] frequency (MHz)	Observed[1] T_{MB} (K)	Model[2] T_{MB} (K)	Blends
tEME-EE’	$15_{0,15}$–$14_{1,14}$	106 667.388	46.1	9.41	†			
tEME-EE	$21_{3,18}$–$21_{2,19}$	109 216.897	99.8	12.35	109 215.1	0.02	0.01	U-line
tEME-EE’	$21_{3,18}$–$21_{2,19}$	109 216.904	99.8	12.35	†			
tEME-AE	$21_{3,18}$–$21_{2,19}$	109 217.159	99.8	12.35	†			
tEME-EA	$21_{3,18}$–$21_{2,19}$	109 219.323	99.8	12.35	109 219.6	0.01	0.01	
tEME-AA	$21_{3,18}$–$21_{2,19}$	109 219.581	99.8	12.35	†			
tEME-EE	$20_{3,17}$–$20_{2,18}$	110 694.695	91.6	11.56	…	…	0.02	CH_3CN $v_8 = 1$
tEME-EE’	$20_{3,17}$–$20_{2,18}$	110 694.705	91.6	11.56	†			
tEME-AE	$20_{3,17}$–$20_{2,18}$	110 694.963	91.6	11.56	†			
tEME-EA	$20_{3,17}$–$20_{2,18}$	110 697.132	91.6	11.56	…	…	0.01	CH_3CN $v_8 = 1$
tEME-AA	$20_{3,17}$–$20_{2,18}$	110 697.395	91.6	11.56	†			
tEME-EE’	$12_{1,12}$–$11_{0,11}$	111 178.747	30.8	7.46	111 178.7	0.03	0.02	
tEME-EE	$12_{1,12}$–$11_{0,11}$	111 178.747	30.8	7.46	†			
tEME-AE	$12_{1,12}$–$11_{0,11}$	111 178.796	30.8	7.46	†			
tEME-EA	$12_{1,12}$–$11_{0,11}$	111 179.248	30.8	7.46	†			
tEME-AA	$12_{1,12}$–$11_{0,11}$	111 179.297	30.8	7.46	†			
tEME-EE	$19_{3,16}$–$19_{2,17}$	112 072.074	83.9	10.80	112 072.3	0.03	0.02	
tEME-EE’	$19_{3,16}$–$19_{2,17}$	112 072.088	83.9	10.80	†			
tEME-AE	$19_{3,16}$–$19_{2,17}$	112 072.349	83.9	10.80	†			
tEME-EA	$19_{3,16}$–$19_{2,17}$	112 074.518	83.9	10.80	112 074.5	0.03	0.01	
tEME-AA	$19_{3,16}$–$19_{2,17}$	112 074.786	83.9	10.80	†			
tEME-EE	$18_{3,15}$–$18_{2,16}$	113 336.061	76.5	10.08	113 336.2	0.02	0.02	
tEME-EE’	$18_{3,15}$–$18_{2,16}$	113 336.081	76.5	10.08	†			
tEME-AE	$18_{3,15}$–$18_{2,16}$	113 336.343	76.5	10.08	†			
tEME-EA	$18_{3,15}$–$18_{2,16}$	113 338.507	76.5	10.08	113 338.7	0.03	0.01	$CH_2^{13}CHCN$
tEME-AA	$18_{3,15}$–$18_{2,16}$	113 338.779	76.5	10.08	†			
tEME-EE	$17_{3,14}$–$17_{2,15}$	114 477.615	69.5	9.39	114 477.9	0.05	0.02	U-line
tEME-EE’	$17_{3,14}$–$17_{2,15}$	114 477.643	69.5	9.39	†			
tEME-AE	$17_{3,14}$–$17_{2,15}$	114 477.905	69.5	9.39	†			
tEME-EA	$17_{3,14}$–$17_{2,15}$	114 480.057	69.5	9.39	…	…	0.01	CH_3COOCH_3
tEME-AA	$17_{3,14}$–$17_{2,15}$	114 480.333	69.5	9.39	†			
tEME-AE	$20_{1,19}$–$19_{2,18}$	114 717.852	83.4	6.11	114 718.0	0.06	0.01	CH_3CHO $v_t = 1$
tEME-EE	$20_{1,19}$–$19_{2,18}$	114 717.961	83.4	6.11	†			
tEME-EE’	$20_{1,19}$–$19_{2,18}$	114 717.962	83.4	6.11	†			
tEME-EE	$16_{3,13}$–$16_{2,14}$	115 491.673	62.9	8.73	…	…	0.02	CH_3CHO
tEME-EE’	$16_{3,13}$–$16_{2,14}$	115 491.713	62.9	8.73	†			
tEME-AE	$16_{3,13}$–$16_{2,14}$	115 491.972	62.9	8.73	†			
tEME-EA	$16_{3,13}$–$16_{2,14}$	115 494.106	62.9	8.73	…	…	0.02	CH_3CHO
tEME-AA	$16_{3,13}$–$16_{2,14}$	115 494.385	62.9	8.73	†			
tEME-AA	$16_{0,16}$–$15_{1,15}$	115 618.006	52.2	10.34	115 618.4	0.07	0.04	
tEME-EA	$16_{0,16}$–$15_{1,15}$	115 618.033	52.2	10.34	†			

Species	Transition $J_{K_a,K_c} - J'_{K'_a,K'_c}$	Predicted frequency (MHz)	E_{upp} (K)	S_{ij}	Observed[1] frequency (MHz)	Observed[1] T_{MB} (K)	Model[2] T_{MB} (K)	Blends
tEME-AE	$16_{0,16}$–$15_{1,15}$	115 618.391	52.2	10.34	†			
tEME-EE	$16_{0,16}$–$15_{1,15}$	115 618.417	52.2	10.34	†			
tEME-EE’	$16_{0,16}$–$15_{1,15}$	115 618.417	52.2	10.34	†			
tEME-EE’	$19_{3,17}$–$19_{2,18}$	123 318.746	83.8	10.04	123 318.8	0.02	0.02	
tEME-EE	$19_{3,17}$–$19_{2,18}$	123 318.760	83.8	10.04	†			
tEME-AE	$19_{3,17}$–$19_{2,18}$	123 319.043	83.8	10.04	†			
tEME-EA	$19_{3,17}$–$19_{2,18}$	123 321.168	83.8	10.04	123 321.3	0.04	0.01	$CH_3O^{13}COH$
tEME-AA	$19_{3,17}$–$19_{2,18}$	123 321.458	83.8	10.04	†			
tEME-EE’	$20_{3,18}$–$20_{2,19}$	124 043.337	91.6	10.58	124 043.5	0.03	0.02	$CH_3COOH v_t = 1$
tEME-EE	$20_{3,18}$–$20_{2,19}$	124 043.347	91.6	10.58	†			
tEME-AE	$20_{3,18}$–$20_{2,19}$	124 043.631	91.6	10.58	†			
tEME-EA	$20_{3,18}$–$20_{2,19}$	124 045.738	91.6	10.58	124 046.0	0.02	0.01	
tEME-AA	$20_{3,18}$–$20_{2,19}$	124 046.027	91.6	10.58	†			
tEME-AA	$17_{0,17}$–$16_{1,16}$	124 519.803	58.7	11.29	124 519.5	0.19	0.05	U-line
tEME-EA	$17_{0,17}$–$16_{1,16}$	124 519.826	58.7	11.29	†			
tEME-AE	$17_{0,17}$–$16_{1,16}$	124 520.163	58.7	11.29	†			
tEME-EE	$17_{0,17}$–$16_{1,16}$	124 520.186	58.7	11.29	†			
tEME-EE’	$17_{0,17}$–$16_{1,16}$	124 520.186	58.7	11.29	†			
tEME-EE’	$14_{1,14}$–$13_{0,13}$	124 648.594	41.0	9.02	124 649.0	0.06	0.04	
tEME-EE	$14_{1,14}$–$13_{0,13}$	124 648.594	41.0	9.02	†			
tEME-AE	$14_{1,14}$–$13_{0,13}$	124 648.637	41.0	9.02	†			
tEME-EA	$14_{1,14}$–$13_{0,13}$	124 649.062	41.0	9.02	†			
tEME-AA	$14_{1,14}$–$13_{0,13}$	124 649.106	41.0	9.02	†			
tEME-EE’	$21_{3,19}$–$21_{2,20}$	124 866.195	99.7	11.10	…	…	0.02	SO_2
tEME-EE	$21_{3,19}$–$21_{2,20}$	124 866.202	99.7	11.10	†			
tEME-AE	$21_{3,19}$–$21_{2,20}$	124 866.487	99.7	11.10	†			
tEME-EA	$21_{3,19}$–$21_{2,20}$	124 868.576	99.7	11.10	…	…	0.01	SO_2
tEME-AA	$21_{3,19}$–$21_{2,20}$	124 868.864	99.7	11.10	†			
tEME-AA	$21_{1,20}$–$20_{2,19}$	125 001.226	91.6	6.68	…	…	0.01	CH_3OCOH
tEME-EA	$21_{1,20}$–$20_{2,19}$	125 001.329	91.6	6.68	†			
tEME-AE	$21_{1,20}$–$20_{2,19}$	125 002.535	91.6	6.68	…	…	0.02	CH_3OCOH
tEME-EE	$21_{1,20}$–$20_{2,19}$	125 002.638	91.6	6.68	†			
tEME-EE’	$21_{1,20}$–$20_{2,19}$	125 002.638	91.6	6.68	†			
tEME-EE’	$7_{2,6}$–$6_{1,5}$	125 433.445	15.4	2.61	…	…	0.01	CH_3CH_2CN, SO_2
tEME-EE	$7_{2,6}$–$6_{1,5}$	125 433.472	15.4	2.61	†			
tEME-AE	$7_{2,6}$–$6_{1,5}$	125 433.646	15.4	2.61	†			
tEME-EE’	$22_{3,20}$–$22_{2,21}$	125 793.386	108.2	11.61	…	…	0.02	CH_3CH_2CN v_{13}/v_{21}
tEME-EE	$22_{3,20}$–$22_{2,21}$	125 793.392	108.2	11.61	†			
tEME-AE	$22_{3,20}$–$22_{2,21}$	125 793.677	108.2	11.61	†			
tEME-EA	$22_{3,20}$–$22_{2,21}$	125 795.748	108.2	11.61	…	…	0.01	CH_3CH_2CN v_{13}/v_{21}
tEME-AA	$22_{3,20}$–$22_{2,21}$	125 796.036	108.2	11.61	†			

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Species	**Transition** $J_{K_a,K_c} - J'_{K'_a,K'_c}$	**Predicted frequency (MHz)**	E_{upp} **(K)**	S_{ij}	**Observed[1] frequency (MHz)**	**Observed[1]** T_{MB} **(K)**	**Model[2]** T_{MB} **(K)**	**Blends**
tEME-EE'	$23_{3,21}–23_{2,22}$	126 830.671	117.1	12.11	…	…	0.02	$HC^{13}CCN$
tEME-EE	$23_{3,21}–23_{2,22}$	126 830.675	117.1	12.11	†			
tEME-AE	$23_{3,21}–23_{2,22}$	126 830.960	117.1	12.11	†			
tEME-EA	$23_{3,21}–23_{2,22}$	126 833.013	117.1	12.11	…	…	0.01	$HC^{13}CCN$
tEME-AA	$23_{3,21}–23_{2,22}$	126 833.301	117.1	12.11	†			
tEME-EE'	$24_{3,22}–24_{2,23}$	127 983.452	126.4	12.59	127 983.6	0.07	0.02	U-line
tEME-EE	$24_{3,22}–24_{2,23}$	127 983.456	126.4	12.59	†			
tEME-AE	$24_{3,22}–24_{2,23}$	127 983.741	126.4	12.59	†			
tEME-EA	$24_{3,22}–24_{2,23}$	127 985.776	126.4	12.59	127 986.1	0.06	0.01	NH_2CHO $v_{12} = 1$
tEME-AA	$24_{3,22}–24_{2,23}$	127 986.063	126.4	12.59	†			
tEME-EE'	$25_{3,23}–25_{2,24}$	129 256.739	136.1	13.06	129 256.8	0.04	0.02	
tEME-EE	$25_{3,23}–25_{2,24}$	129 256.741	136.1	13.06	†			
tEME-AE	$25_{3,23}–25_{2,24}$	129 257.027	136.1	13.06	†			
tEME-EA	$25_{3,23}–25_{2,24}$	129 259.044	136.1	13.06	129 259.3	0.04	0.01	
tEME-AA	$25_{3,23}–25_{2,24}$	129 259.331	136.0	13.06	†			
tEME-EE'	$26_{3,24}–26_{2,25}$	130 655.101	146.1	13.52	…	…	0.02	U-line
tEME-EE	$26_{3,24}–26_{2,25}$	130 655.103	146.1	13.52	†			
tEME-AE	$26_{3,24}–26_{2,25}$	130 655.389	146.1	13.52	†			
tEME-EA	$26_{3,24}–26_{2,25}$	130 657.388	146.1	13.52	…	…	0.01	U-line
tEME-AA	$26_{3,24}–26_{2,25}$	130 657.674	146.1	13.52	†			
tEME-EE'	$15_{1,15}–14_{0,14}$	131 372.619	46.7	9.86	131 372.7	0.05	0.05	
tEME-EE	$15_{1,15}–14_{0,14}$	131 372.619	46.7	9.86	†			
tEME-AE	$15_{1,15}–14_{0,14}$	131 372.660	46.7	9.86	†			
tEME-EA	$15_{1,15}–14_{0,14}$	131 373.069	46.7	9.86	†			
tEME-AA	$15_{1,15}–14_{0,14}$	131 373.110	46.7	9.86	†			
tEME-EE'	$27_{3,25}–27_{2,26}$	132 182.639	156.6	13.95	132 182.8	0.04	0.02	
tEME-EE	$27_{3,25}–27_{2,26}$	132 182.640	156.6	13.95	†			
tEME-AE	$27_{3,25}–27_{2,26}$	132 182.927	156.6	13.95	†			
tEME-EA	$27_{3,25}–27_{2,26}$	132 184.906	156.6	13.95	132 185.5	0.01	0.01	
tEME-AA	$27_{3,25}–27_{2,26}$	132 185.194	156.6	13.95	†			
tEME-EE'	$8_{2,7}–7_{1,6}$	132 547.336	18.5	2.87	132 547.2	0.02	0.02	
tEME-EE	$8_{2,7}–7_{1,6}$	132 547.352	18.5	2.87	†			
tEME-AE	$8_{2,7}–7_{1,6}$	132 547.529	18.5	2.87	†			
tEME-EA	$8_{2,7}–7_{1,6}$	132 548.982	18.5	2.87	132 549.0	0.02	0.01	
tEME-AA	$8_{2,7}–7_{1,6}$	132 549.167	18.5	2.87	†			
tEME-AA	$18_{0,18}–17_{1,17}$	133 362.763	65.6	12.27	…	…	0.06	$O^{13}CS$, CH_2CHCN $v_{11} = 1$
tEME-EA	$18_{0,18}–17_{1,17}$	133 362.784	65.6	12.27	†			
tEME-AE	$18_{0,18}–17_{1,17}$	133 363.098	65.6	12.27	†			
tEME-EE	$18_{0,18}–17_{1,17}$	133 363.118	65.6	12.27	†			
tEME-EE'	$18_{0,18}–17_{1,17}$	133 363.118	65.6	12.27	†			
tEME-EE'	$28_{3,26}–28_{2,27}$	133 842.950	167.4	14.37	…	…	0.02	CH_2DOH

Species	Transition $J_{K_a,K_c} - J'_{K'_a,K'_c}$	Predicted frequency (MHz)	E_{upp} (K)	S_{ij}	Observed[1] frequency (MHz)	Observed[1] T_{MB} (K)	Model[2] T_{MB} (K)	Blends
tEME-EE	$28_{3,26}$–$28_{2,27}$	133 842.951	167.4	14.37	†			
tEME-AE	$28_{3,26}$–$28_{2,27}$	133 843.238	167.4	14.37	†			
tEME-EA	$28_{3,26}$–$28_{2,27}$	133 845.198	167.4	14.37	…	…	0.01	CH_2DOH
tEME-AA	$28_{3,26}$–$28_{2,27}$	133 845.486	167.4	14.37	†			
tEME-AA	$22_{1,21}$–$21_{2,20}$	135 315.986	100.2	7.28	135 316.0	0.07	0.01	U-line
tEME-EA	$22_{1,21}$–$21_{2,20}$	135 316.082	100.2	7.28	†			
tEME-AE	$22_{1,21}$–$21_{2,20}$	135 317.259	100.2	7.28	135 317.5	0.05	0.02	CH_3CHO $v_t = 1$
tEME-EE	$22_{1,21}$–$21_{2,20}$	135 317.355	100.2	7.28	†			
tEME-EE’	$22_{1,21}$–$21_{2,20}$	135 317.355	100.2	7.28	†			
tEME-EE’	$29_{3,27}$–$29_{2,28}$	135 639.103	178.6	14.77	…	…	0.02	CH_3OCOH $v_t = 1$
tEME-EE	$29_{3,27}$–$29_{2,28}$	135 639.104	178.6	14.77	†			
tEME-AE	$29_{3,27}$–$29_{2,28}$	135 639.392	178.6	14.77	†			
tEME-EA	$29_{3,27}$–$29_{2,28}$	135 641.333	178.6	14.77	…	…	0.01	CH_3OCOH $v_t = 1$
tEME-AA	$29_{3,27}$–$29_{2,28}$	135 641.621	178.6	14.77	†			
tEME-EE’	$30_{3,28}$–$30_{2,29}$	137 573.618	190.2	15.14	137 573.7	0.04	0.02	
tEME-EE	$30_{3,28}$–$30_{2,29}$	137 573.618	190.2	15.14	†			
tEME-AE	$30_{3,28}$–$30_{2,29}$	137 573.907	190.2	15.14	†			
tEME-EA	$30_{3,28}$–$30_{2,29}$	137 575.829	190.2	15.14	137 575.9	0.05	0.02	CH_3COOCH_3
tEME-AA	$30_{3,28}$–$30_{2,29}$	137 576.118	190.2	15.14	†			
tEME-EE’	$16_{1,16}$–$15_{0,15}$	138 109.231	52.7	10.73	138 109.7	0.06	0.06	
tEME-EE	$16_{1,16}$–$15_{0,15}$	138 109.231	52.7	10.73	†			
tEME-AE	$16_{1,16}$–$15_{0,15}$	138 109.269	52.7	10.73	†			
tEME-EA	$16_{1,16}$–$15_{0,15}$	138 109.661	52.7	10.73	†			
tEME-AA	$16_{1,16}$–$15_{0,15}$	138 109.699	52.7	10.73	†			
tEME-EE’	$9_{2,8}$–$8_{1,7}$	139 530.181	22.0	3.15	…	…	0.02	CH_2DCN
tEME-EE	$9_{2,8}$–$8_{1,7}$	139 530.191	22.0	3.15	†			
tEME-AE	$9_{2,8}$–$8_{1,7}$	139 530.369	22.0	3.15	†			
tEME-EA	$9_{2,8}$–$8_{1,7}$	139 531.807	22.0	3.15	…	…	0.01	CH_2DCN
tEME-AA	$9_{2,8}$–$8_{1,7}$	139 531.989	22.0	3.15	†			
tEME-EE’	$31_{3,29}$–$31_{2,30}$	139 648.445	202.2	15.50	…	…	0.02	CH_3COCH_3
tEME-EE	$31_{3,29}$–$31_{2,30}$	139 648.445	202.2	15.50	†			
tEME-AE	$31_{3,29}$–$31_{2,30}$	139 648.735	202.2	15.50	†			
tEME-EA	$31_{3,29}$–$31_{2,30}$	139 650.637	202.2	15.50	…	…	0.01	CH_3COCH_3
tEME-AA	$31_{3,29}$–$31_{2,30}$	139 650.927	202.2	15.50	†			
tEME-EE	$8_{2,6}$–$7_{1,7}$	140 527.950	18.5	2.43	140 528.1	0.02	0.02	
tEME-EE’	$8_{2,6}$–$7_{1,7}$	140 527.966	18.5	2.43	†			
tEME-AE	$8_{2,6}$–$7_{1,7}$	140 528.160	18.5	2.43	†			
tEME-EA	$8_{2,6}$–$7_{1,7}$	140 529.589	18.5	2.43	140 529.6	0.03	0.01	U-line
tEME-AA	$8_{2,6}$–$7_{1,7}$	140 529.791	18.5	2.43	†			
tEME-EE’	$32_{3,30}$–$32_{2,31}$	141 864.954	214.6	15.83	…	…	0.02	CH_3COOH $v_t = 1$
tEME-EE	$32_{3,30}$–$32_{2,31}$	141 864.954	214.6	15.83	†			

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Species	**Transition** $J_{K_a,K_c} - J'_{K'_a,K'_c}$	**Predicted frequency (MHz)**	E_{upp} **(K)**	S_{ij}	**Observed frequency (MHz)**[1]	**Observed** T_{MB} **(K)**[1]	**Model** T_{MB} **(K)**[2]	**Blends**
tEME-AE	$32_{3,30}$–$32_{2,31}$	141 865.246	214.6	15.83	†			
tEME-EA	$32_{3,30}$–$32_{2,31}$	141 867.127	214.6	15.83	…	…	0.01	CH_3COOH v_t = 1
tEME-AA	$32_{3,30}$–$32_{2,31}$	141 867.419	214.6	15.83	†			
tEME-AA	$19_{0,19}$–$18_{1,18}$	142 139.587	72.8	13.27	142 139.7	0.08	0.06	
tEME-EA	$19_{0,19}$–$18_{1,18}$	142 139.605	72.8	13.27	†			
tEME-AE	$19_{0,19}$–$18_{1,18}$	142 139.896	72.8	13.27	†			
tEME-EE	$19_{0,19}$–$18_{1,18}$	142 139.914	72.8	13.27	†			
tEME-EE’	$19_{0,19}$–$18_{1,18}$	142 139.914	72.8	13.27	†			
tEME-EE’	$3_{3,1}$–$2_{2,1}$	143 977.261	12.7	2.45	143 977.8	0.06	0.02	U-line
tEME-EE	$3_{3,1}$–$2_{2,1}$	143 977.759	12.7	2.41	†			
tEME-AE	$3_{3.1}$–$2_{2.1}$	143 977.810	12.7	2.44	†			
tEME-EA	$3_{3,1}$–$2_{2,0}$	143 979.010	12.7	.72	143 980.0	0.05	0.02	CH_3COCH_3
tEME-EE	$3_{3,0}$–$2_{2,0}$	143 979.276	12.7	2.41	†			
tEME-EE’	$3_{3,0}$–$2_{2,0}$	143 979.774	12.7	2.45	†			
tEME-AE	$3_{3,0}$–$2_{2,0}$	143 979.832	12.7	2.44	†			
tEME-AA	$3_{3,1}$–$2_{2,0}$	143 980.192	12.7	2.50	†			
tEME-EA	$3_{3,0}$–$2_{2,0}$	143 980.533	12.7	1.78	†			
tEME-EE’	$33_{3,31}$–$33_{2,32}$	144 223.924	227.3	16.14	144 224.0	0.02	0.01	
tEME-EE	$33_{3,31}$–$33_{2,32}$	144 223.925	227.3	16.14	†			
tEME-AE	$33_{3,31}$–$33_{2,32}$	144 224.218	227.3	16.14	†			
tEME-EE’	$17_{1,17}$–$16_{0,16}$	144 871.829	59.2	11.63	144 872.1	0.06	0.06	
tEME-EE	$17_{1,17}$–$16_{0,16}$	144 871.829	59.2	11.63	†			
tEME-AE	$17_{1,17}$–$16_{0,16}$	144 871.864	59.2	11.63	†			
tEME-EA	$17_{1,17}$–$16_{0,16}$	144 872.238	59.2	11.63	†			
tEME-AA	$17_{1,17}$–$16_{0,16}$	144 872.273	59.2	11.63	†			
tEME-AA	$23_{1,22}$–$22_{2,21}$	145 647.137	109.2	7.92	145 647.4	0.03	0.01	
tEME-EA	$23_{1,22}$–$22_{2,21}$	145 647.226	109.2	7.92	†			
tEME-AE	$23_{1,22}$–$22_{2,21}$	145 648.372	109.2	7.92	145 648.6	0.03	0.02	
tEME-EE	$23_{1,22}$–$22_{2,21}$	145 648.461	109.2	7.92	†			
tEME-EE’	$23_{1,22}$–$22_{2,21}$	145 648.462	109.2	7.92	†			
tEME-EE’	$10_{2,9}$–$9_{1,8}$	146 383.619	25.8	3.44	146 384.0	0.03	0.02	
tEME-EE	$10_{2,9}$–$9_{1,8}$	146 383.626	25.8	3.44	†			
tEME-AE	$10_{2,9}$–$9_{1,8}$	146 383.802	25.8	3.44	†			
tEME-EA	$10_{2,9}$–$9_{1,8}$	146 385.228	25.8	3.44	146 385.5	0.03	0.02	
tEME-AA	$10_{2,9}$–$9_{1,8}$	146 385.408	25.8	3.44	†			
tEME-EE	$36_{4,32}$–$36_{3,33}$	146 397.039	276.3	21.88	…	…	0.01	SO_2, CH_3OCH_3
tEME-EE’	$36_{4,32}$–$36_{3,33}$	146 397.042	276.3	21.88	†			
tEME-AE	$36_{4,32}$–$36_{3,33}$	146 397.310	276.3	21.88	†			
tEME-EE’	$34_{3,32}$–$34_{2,33}$	146 725.545	240.5	16.44	146 725.6	0.03	0.01	$SO^{18}O$
tEME-EE	$34_{3,32}$–$34_{2,33}$	146 725.545	240.5	16.44	†			
tEME-AE	$34_{3,32}$–$34_{2,33}$	146 725.840	240.5	16.44	†			

Species	Transition $J_{K_a,K_c} - J'_{K'_a,K'_c}$	Predicted frequency (MHz)	E_{upp} (K)	S_{ij}	Observed[1] frequency (MHz)	Observed[1] T_{MB} (K)	Model[2] T_{MB} (K)	Blends
tEME-AE	$29_{2,27}$–$28_{3,26}$	146 736.865	174.4	6.43	…	…	0.01	U-line
tEME-EE	$29_{2,27}$–$28_{3,26}$	146 737.046	174.4	6.43	†			
tEME-EE’	$29_{2,27}$–$28_{3,26}$	146 737.048	174.4	6.43	†			
tEME-EE	$35_{4,31}$–$35_{3,32}$	148 578.427	262.3	20.95	…	…	0.01	CH_3OCOH v_t = 1
tEME-EE’	$35_{4,31}$–$35_{3,32}$	148 578.431	262.3	20.95	†			
tEME-AE	$35_{4,31}$–$35_{3,32}$	148 578.707	262.3	20.95	†			
tEME-EE’	$35_{3,33}$–$35_{2,34}$	149 369.412	254.0	16.71	…	…	0.01	CH_3OCOH v_t = 1
tEME-EE	$35_{3,33}$–$35_{2,34}$	149 369.412	254.0	16.71	†			
tEME-AE	$35_{3,33}$–$35_{2,34}$	149 369.709	254.0	16.71	†			
tEME-EE	$9_{2,7}$–$8_{1,8}$	149 921.139	22.0	2.54	…	…	0.02	CH_3OCOH
tEME-EE’	$9_{2,7}$–$8_{1,8}$	149 921.149	22.0	2.54	†			
tEME-AE	$9_{2,7}$–$8_{1,8}$	149 921.348	22.0	2.54	†			
tEME-EA	$9_{2,7}$–$8_{1,8}$	149 922.787	22.0	2.54	…	…	0.01	CH_3OCOH
tEME-AA	$9_{2,7}$–$8_{1,8}$	149 922.992	22.0	2.54	†			
tEME-EE	$34_{4,30}$–$34_{3,31}$	150 661.347	248.7	20.06	150 661.4	0.04	0.02	U-line
tEME-EE’	$34_{4,30}$–$34_{3,31}$	150 661.353	248.7	20.06	†			
tEME-AE	$34_{4,30}$–$34_{3,31}$	150 661.636	248.7	20.06	†			
tEME-EA	$34_{4,30}$–$34_{3,31}$	150 664.261	248.7	20.06	150 664.4	0.03	0.02	U-line
tEME-AA	$34_{4,30}$–$34_{3,31}$	150 664.547	248.7	20.06	†			
tEME-AA	$20_{0,20}$–$19_{1,19}$	150 845.281	80.4	14.28	150 845.4	0.08	0.09	
tEME-EA	$20_{0,20}$–$19_{1,19}$	150 845.296	80.4	14.28	†			
tEME-AE	$20_{0,20}$–$19_{1,19}$	150 845.565	80.4	14.28	†			
tEME-EE	$20_{0,20}$–$19_{1,19}$	150 845.580	80.4	14.28	†			
tEME-EE’	$20_{0,20}$–$19_{1,19}$	150 845.580	80.4	14.28	†			
tEME-EE’	$18_{1,18}$–$17_{0,17}$	151 672.109	66.0	12.56	151 672.4	0.06	0.09	
tEME-EE	$18_{1,18}$–$17_{0,17}$	151 672.109	66.0	12.56	†			
tEME-AE	$18_{1,18}$–$17_{0,17}$	151 672.141	66.0	12.56	†			
tEME-EA	$18_{1,18}$–$17_{0,17}$	151 672.495	66.0	12.56	†			
tEME-AA	$18_{1,18}$–$17_{0,17}$	151 672.527	66.0	12.56	†			
tEME-EE’	$11_{2,10}$–$10_{1,9}$	153 109.700	30.1	3.73	153 109.7	0.05	0.03	
tEME-EE	$11_{2,10}$–$10_{1,9}$	153 109.705	30.1	3.73	†			
tEME-AE	$11_{2,10}$–$10_{1,9}$	153 109.879	30.1	3.73	†			
tEME-EA	$11_{2,10}$–$10_{1,9}$	153 111.294	30.1	3.73	153 111.4	0.05	0.02	U-line
tEME-AA	$11_{2,10}$–$10_{1,9}$	153 111.471	30.1	3.73	†			
tEME-EE	$32_{4,28}$–$32_{3,29}$	154 467.850	222.8	18.42	154 468.1	0.02	0.02	
tEME-EE’	$32_{4,28}$–$32_{3,29}$	154 467.860	222.8	18.42	†			
tEME-AE	$32_{4,28}$–$32_{3,29}$	154 468.157	222.8	18.42	†			
tEME-AA	$24_{1,23}$–$23_{2,22}$	155 980.202	118.5	8.61	…	…	0.03	CH_3CH_2CN v_{12} = 1
tEME-EA	$24_{1,23}$–$23_{2,22}$	155 980.284	118.5	8.61	†			
tEME-AE	$24_{1,23}$–$23_{2,22}$	155 981.396	118.5	8.61	…	…	0.03	CH_3CH_2CN v_{12} = 1
tEME-EE	$24_{1,23}$–$23_{2,22}$	155 981.478	118.5	8.61	†			

Species	Transition $J_{K_a,K_c} - J'_{K'_a,K'_c}$	Predicted frequency (MHz)	E_{upp} (K)	S_{ij}	Observed[1] frequency (MHz)	Observed[1] T_{MB} (K)	Model[2] T_{MB} (K)	Blends
tEME-EE'	$24_{1,23}–23_{2,22}$	155 981.479	118.5	8.61	†			
tEME-EE	$31_{4,27}–31_{3,28}$	156 169.103	210.3	17.65	…	…	0.02	CH_3CH_2CN
tEME-EE'	$31_{4,27}–31_{3,28}$	156 169.114	210.3	17.65	†			
tEME-AE	$31_{4,27}–31_{3,28}$	156 169.418	210.3	17.65	†			
tEME-EE	$30_{4,26}–31_{3,27}$	157 727.158	198.3	16.91	157 727.3	0.03	0.02	
tEME-EE'	$30_{4,26}–31_{3,27}$	157 727.174	198.3	16.91	†			
tEME-AE	$30_{4,26}–31_{3,27}$	157 727.482	198.3	16.91	†			
tEME-EE'	$19_{1,19}–18_{0,18}$	158 519.756	73.2	13.52	…	…	0.10	CH_3OCOH $v_t = 1$, CH_3COCH_3
tEME-EE	$19_{1,19}–18_{0,18}$	158 519.756	73.2	13.52	†			
tEME-AE	$19_{1,19}–18_{0,18}$	158 519.786	73.2	13.52	†			
tEME-EA	$19_{1,19}–18_{0,18}$	158 520.119	73.2	13.52	†			
tEME-AA	$19_{1,19}–18_{0,18}$	158 520.149	73.2	13.52	†			
tEME-EE	$29_{4,25}–29_{3,26}$	159 140.100	186.7	16.20	…	…	0.03	U-line
tEME-EE'	$29_{4,25}–29_{3,26}$	159 140.121	186.7	16.19	†			
tEME-AE	$29_{4,25}–29_{3,26}$	159 140.432	186.7	16.20	†			
tEME-EA	$29_{4,25}–29_{3,26}$	159 143.035	186.7	16.20	…	…	0.02	U-line
tEME-AA	$29_{4,25}–29_{3,26}$	159 143.357	186.7	16.20	†			
tEME-AA	$21_{0,21}–20_{1,20}$	159 477.061	88.4	15.31	159 477.1	0.15	0.10	CH_2CN
tEME-EA	$21_{0,21}–20_{1,20}$	159 477.074	88.4	15.31	†			
tEME-AE	$21_{0,21}–20_{1,20}$	159 477.319	88.4	15.31	†			
tEME-EE	$21_{0,21}–20_{1,20}$	159 477.332	88.4	15.31	†			
tEME-EE'	$21_{0,21}–20_{1,20}$	159 477.332	88.4	15.31	†			
tEME-EE	$10_{2,8}–9_{1,9}$	159 548.654	25.9	2.61	159 548.8	0.09	0.02	CH_3COOH $v_t = 2$
tEME-EE'	$10_{2,8}–9_{1,9}$	159 548.661	25.9	2.61	†	”	”	
tEME-AE	$10_{2,8}–9_{1,9}$	159 548.866	25.9	2.61	†	”	”	
tEME-EE'	$12_{2,11}–11_{1,10}$	159 710.946	34.7	4.05	…	…	0.03	CH_3CH_2CN v_{12}/v_{21}
tEME-EE	$12_{2,11}–11_{1,10}$	159 710.950	34.7	4.05	†			
tEME-AE	$12_{2,11}–11_{1,10}$	159 711.121	34.7	4.05	†			
tEME-EA	$12_{2,11}–11_{1,10}$	159 712.526	34.7	4.05	…	…	0.02	CH_3CH_2CN v_{12}/v_{21}
tEME-AA	$12_{2,11}–11_{1,10}$	159 712.699	34.7	4.05	†			
tEME-EE	$28_{4,24}–28_{3,25}$	160 409.193	175.5	15.50	…	…	0.03	CH_3COCH_3
tEME-EE'	$28_{4,24}–28_{3,25}$	160 409.221	175.5	15.50	†			
tEME-AE	$28_{4,24}–28_{3,25}$	160 409.535	175.5	15.50	†			
tEME-EA	$28_{4,24}–28_{3,25}$	160 412.123	175.5	15.50	…	…	0.02	CH_3OCOH $v_t = 1$
tEME-AA	$28_{4,24}–28_{3,25}$	160 412.450	175.5	15.50	†			
tEME-EE'	$10_{3,8}–9_{2,7}$	199 842.884	31.6	3.55	199 843.5	…	0.05	CH_3OCOH $v_t = 2$
tEME-EE	$10_{3,8}–9_{2,7}$	199 843.513	31.6	3.65	†			
tEME-AE	$10_{3,8}–9_{2,7}$	199 843.521	31.6	3.61	†			
tEME-EA	$10_{3,8}–9_{2,7}$	199 846.703	31.6	3.78	…	…	0.04	CH_3OCOH $v_t = 1$
tEME-AA	$10_{3,8}–9_{2,7}$	199 847.033	31.6	3.78	†			
tEME-EE'	$4_{4,1}–3_{3,1}$	199 953.072	22.3	3.50	199 953.5	0.18	0.06	CH_3CH_2OH

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Species	Transition $J_{K_a,K_c} - J'_{K'_a,K'_c}$	Predicted frequency (MHz)	E_{upp} (K)	S_{ij}	Observed[1] frequency (MHz)	Observed[1] T_{MB} (K)	Model[2] T_{MB} (K)	Blends
tEME-EE	$4_{4,1}$–$3_{3,1}$	199 953.406	22.3	3.50	†			
tEME-AE	$4_{4,1}$–$3_{3,1}$	199 953.633	22.3	3.50	†			
tEME-EE	$4_{4,0}$–$3_{3,0}$	199 954.307	22.3	3.50	199 954.7	0.12	0.06	CH_3CH_2OH
tEME-EE’	$4_{4,0}$–$3_{3,0}$	199 954.642	22.3	3.50	†			
tEME-AE	$4_{4,0}$–$3_{3,0}$	199 954.869	22.3	3.50	†			
tEME-EA	$4_{4,1}$–$3_{3,1}$	199 956.750	22.3	3.50	199 957.2	0.19	0.08	CH_2CHCN $v_{15} = 1$
tEME-EA	$4_{4,0}$–$3_{3,0}$	199 957.085	22.3	3.50	†			
tEME-AA	$4_{4,1}$–$3_{3,0}$	199 957.305	22.3	3.50	†			
tEME-AA	$4_{4,0}$–$3_{3,1}$	199 957.317	22.3	3.50	†			
tEME-EE	$10_{3,7}$–$9_{2,8}$	200 603.336	31.6	3.64	…	…	0.05	U-line
tEME-AE	$10_{3,7}$–$9_{2,8}$	200 603.932	31.6	3.59	†			
tEME-EE’	$10_{3,7}$–$9_{2,8}$	200 603.965	31.6	3.54	†			
tEME-EA	$10_{3,7}$–$9_{2,8}$	200 605.130	31.6	3.76	…	…	0.04	CH_3OCOH
tEME-AA	$10_{3,7}$–$9_{2,8}$	200 605.404	31.6	3.77	†			
tEME-EE	$14_{2,12}$–$13_{1,13}$	200 820.096	45.3	2.62	…	…	0.04	CH_3OH
tEME-EE’	$14_{2,12}$–$13_{1,13}$	200 820.098	45.3	2.62	†			
tEME-AE	$14_{2,12}$–$13_{1,13}$	200 820.324	45.3	2.62	†			
tEME-EA	$14_{2,12}$–$13_{1,13}$	200 821.765	45.3	2.62	…	…	0.03	CH_3OH
tEME-AA	$14_{2,12}$–$13_{1,13}$	200 821.991	45.3	2.62	†			
tEME-EE’	$25_{1,25}$–$24_{0,24}$	200 871.974	124.2	19.55	200 872.2	0.59	0.20	CH_2CHCN $v_{11} = 2$
tEME-EE	$25_{1,25}$–$24_{0,24}$	200 871.975	124.2	19.55	†			
tEME-AE	$25_{1,25}$–$24_{0,24}$	200 871.991	124.2	19.55	†			
tEME-EA	$25_{1,25}$–$24_{0,24}$	200 872.199	124.2	19.55	†			
tEME-AA	$25_{1,25}$–$24_{0,24}$	200 872.216	124.2	19.55	†			
tEME-AA	$26_{0,26}$–$25_{1,25}$	201 553.272	133.9	20.51	201 553.4	0.32	0.21	
tEME-EA	$26_{0,26}$–$25_{1,25}$	201 553.275	133.9	20.51	†			
tEME-AE	$26_{0,26}$–$25_{1,25}$	201 553.416	133.9	20.51	†			
tEME-EE	$26_{0,26}$–$25_{1,25}$	201 553.419	133.9	20.51	†			
tEME-EE’	$26_{0,26}$–$25_{1,25}$	201 553.419	133.9	20.51	†			
tEME-EE’	$19_{2,18}$–$18_{1,17}$	202 767.815	77.9	6.76	…	…	0.08	$H^{13}CCCN$, CH_3CN $v_8 = 1$
tEME-EE	$19_{2,18}$–$18_{1,17}$	202 767.815	77.9	6.76	†			
tEME-AE	$19_{2,18}$–$18_{1,17}$	202 767.956	77.9	6.76	†			
tEME-EA	$19_{2,18}$–$18_{1,17}$	202 769.267	77.9	6.76	…	…	0.05	$H^{13}CCCN$, CH_3CN $v_8 = 1$
tEME-AA	$19_{2,18}$–$18_{1,17}$	202 769.407	77.9	6.76	†			
tEME-AA	$29_{1,28}$–$28_{2,27}$	207 138.789	170.9	12.63	207 139.6	0.07	0.07	
tEME-EA	$29_{1,28}$–$28_{2,27}$	207 138.838	170.9	12.63	†			
tEME-AE	$29_{1,28}$–$28_{2,27}$	207 139.740	170.9	12.63	†			
tEME-EE	$29_{1,28}$–$28_{2,27}$	207 139.789	170.9	12.63	†			
tEME-EE’	$29_{1,28}$–$28_{2,27}$	207 139.789	170.9	12.63	†			
tEME-EE’	$11_{3,9}$–$10_{2,8}$	207 643.771	35.9	3.90	…	…	0.07	CH_3CH_2CN
tEME-EE	$11_{3,9}$–$10_{2,8}$	207 644.152	35.9	3.94	†			

Species	Transition $J_{K_a,K_c} - J'_{K'_a,K'_c}$	Predicted frequency (MHz)	E_{upp} (K)	S_{ij}	Observed[1] frequency (MHz)	Observed[1] T_{MB} (K)	Model[2] T_{MB} (K)	Blends
tEME-AE	$11_{3,9}–10_{2,8}$	207 644.276	35.9	3.92	†			
tEME-EA	$11_{3,9}–10_{2,8}$	207 647.053	35.9	3.99	207 647.4	0.20	0.05	CH_3CH_2CN
tEME-AA	$11_{3,9}–10_{2,8}$	207 647.369	35.9	3.99	†			
tEME-EE’	$5_{4,2}–4_{3,2}$	208 004.136	24.2	3.60	…	…	0.07	CH_3CH_2CN, CH_3CH_2OH
tEME-EE	$5_{4,2}–4_{3,2}$	208 004.469	24.2	3.60	†			
tEME-AE	$5_{4,2}–4_{3,2}$	208 004.696	24.2	3.60	†			
tEME-EE	$5_{4,1}–4_{3,1}$	208 005.368	24.2	3.60	†			
tEME-EE’	$5_{4,1}–4_{3,1}$	208 005.702	24.2	3.60	†			
tEME-AE	$5_{4,1}–4_{3,1}$	208 005.929	24.2	3.60	†			
tEME-EA	$5_{4,2}–4_{3,2}$	208 007.812	24.2	3.60	…	…	0.09	CH_3CH_2CN, CH_3CH_2OH
tEME-EA	$5_{4,1}–4_{3,1}$	208 008.143	24.2	3.60	†			
tEME-AA	$5_{4,2}–4_{3,1}$	208 008.330	24.2	3.60	†			
tEME-AA	$5_{4,1}–4_{3,2}$	208 008.413	24.2	3.60	†			
tEME-EE’	$26_{1,26}–25_{0,25}$	208 147.627	134.1	20.57	208 147.7	0.58	0.22	CH_2CHCN $v_{11} = 1$
tEME-EE	$26_{1,26}–25_{0,25}$	208 147.627	134.1	20.57	†			
tEME-AE	$26_{1,26}–25_{0,25}$	208 147.642	134.1	20.57	†			
tEME-EA	$26_{1,26}–25_{0,25}$	208 147.831	134.1	20.57	†			
tEME-AA	$26_{1,26}–25_{0,25}$	208 147.846	134.1	20.57	†			
tEME-EE’	$20_{2,19}–19_{1,18}$	208 541.474	85.6	7.24	208 541.5	0.19	0.08	
tEME-EE	$20_{2,19}–19_{1,18}$	208 541.474	85.6	7.24	†			
tEME-AE	$20_{2,19}–19_{1,18}$	208 541.609	85.6	7.24	†			
tEME-EA	$20_{2,19}–19_{1,18}$	208 542.901	85.6	7.24	208 543.0	0.16	0.05	
tEME-AA	$20_{2,19}–19_{1,18}$	208 543.036	85.6	7.24	†			
tEME-EE	$11_{3,8}–10_{2,9}$	208 783.787	35.9	3.92	…	…	0.07	CH_3OCOH
tEME-EE’	$11_{3,8}–10_{2,9}$	208 784.168	35.9	3.88	†			
tEME-AE	$11_{3,8}–10_{2,9}$	208 784.265	35.9	3.90	†			
tEME-EA	$11_{3,8}–10_{2,9}$	208 785.864	35.9	3.96	…	…	0.05	CH_3OCOH
tEME-AA	$11_{3,8}–10_{2,9}$	208 786.150	35.9	3.96	†			
tEME-AA	$27_{0,27}–26_{1,26}$	209 774.111	144.1	21.55	209 774.0	0.35	0.22	CH_2CHCN $v_{15} = 1$
tEME-EA	$27_{0,27}–26_{1,26}$	209 774.113	144.1	21.55	†			
tEME-AE	$27_{0,27}–26_{1,26}$	209 774.236	144.1	21.55	†			
tEME-EE	$27_{0,27}–26_{1,26}$	209 774.238	144.1	21.55	†			
tEME-EE’	$27_{0,27}–26_{1,26}$	209 774.238	144.1	21.55	†			
tEME-EE	$15_{2,13}–14_{1,14}$	211 933.388	51.2	2.56	…	…	0.04	CH_3OCOH
tEME-EE’	$15_{2,13}–14_{1,14}$	211 933.389	51.2	2.56	†			
tEME-AE	$15_{2,13}–14_{1,14}$	211 933.621	51.2	2.56	†			
tEME-EA	$15_{2,13}–14_{1,14}$	211 935.057	51.2	2.56	…	…	0.03	CH_3OCOH
tEME-AA	$15_{2,13}–14_{1,14}$	211 935.290	51.2	2.56	†			
tEME-EE	$32_{5,27}–32_{4,28}$	212 287.353	232.9	17.12	…	…	0.04	CH_3COCH_3
tEME-EE’	$32_{5,27}–32_{4,28}$	212 287.576	232.9	17.07	†			
tEME-AE	$32_{5,27}–32_{4,28}$	212 287.827	232.9	17.10	†			

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Species	Transition $J_{K_a,K_c} - J'_{K'_a,K'_c}$	Predicted frequency (MHz)	E_{upp} (K)	S_{ij}	Observed[1] frequency (MHz)	Observed[1] T_{MB} (K)	Model[2] T_{MB} (K)	Blends
tEME-EA	$32_{5,27}$–$32_{4,28}$	212 290.165	232.9	17.17	…	…	0.03	CH_3COCH_3
tEME-AA	$32_{5,27}$–$32_{4,28}$	212 290.528	232.9	17.17	†			
tEME-EE	$31_{5,26}$–$31_{4,27}$	212 762.787	220.6	16.46	…	…	0.03	CH_3OCH_3
tEME-EE’	$31_{5,26}$–$31_{4,27}$	212 763.095	220.6	16.37	†			
tEME-AE	$31_{5,26}$–$31_{4,27}$	212 763.306	220.6	16.42	†			
tEME-EA	$31_{5,26}$–$31_{4,27}$	212 765.533	220.6	16.55	212 766.9	0.14	0.03	CH_3OCH_3
tEME-AA	$31_{5,26}$–$31_{4,27}$	212 765.897	220.6	16.55	†			
tEME-EE	$30_{5,25}$–$30_{4,26}$	213 178.397	208.6	15.77	…	…	0.04	U-line
tEME-EE’	$30_{5,25}$–$30_{4,26}$	213 178.825	208.6	15.61	†			
tEME-AE	$30_{5,25}$–$30_{4,26}$	213 178.976	208.6	15.70	†			
tEME-EA	$30_{5,25}$–$30_{4,26}$	213 181.046	208.6	15.93	213 181.4	0.21	0.03	CH_2OHCHO
tEME-AA	$30_{5,25}$–$30_{4,26}$	213 181.410	208.6	15.94	†			
tEME-EE’	$33_{5,29}$–$33_{4,30}$	213 495.962	245.7	17.69	213 495.8	0.09	0.04	U-line
tEME-EE	$33_{5,29}$–$33_{4,30}$	213 496.124	245.7	17.72	†			
tEME-AE	$33_{5,29}$–$33_{4,30}$	213 496.418	245.7	17.71	†			
tEME-EA	$33_{5,29}$–$33_{4,30}$	213 499.211	245.7	17.75	213 499.3	0.10	0.03	U-line
tEME-AA	$33_{5,29}$–$33_{4,30}$	213 499.587	245.7	17.75	†			
tEME-EE	$29_{5,24}$–$29_{4,25}$	213 540.983	196.9	15.03	213 541.4	0.16	0.05	CH_2CHCN $v_{11} = 2$
tEME-EE’	$29_{5,24}$–$29_{4,25}$	213 541.573	196.9	14.74	†			
tEME-AE	$29_{5,24}$–$29_{4,25}$	213 541.643	196.9	14.89	†			
tEME-EA	$29_{5,24}$–$29_{4,25}$	213 543.491	196.9	15.32	…	…	0.04	CH_2CHCN $v_{11} = 2$
tEME-AA	$29_{5,24}$–$29_{4,25}$	213 543.850	196.9	15.33	†			
tEME-EE’	$32_{5,28}$–$32_{4,29}$	213 676.308	232.9	17.03	213 676.5	0.20	0.04	CH_3CH_2OH
tEME-EE	$32_{5,28}$–$32_{4,29}$	213 676.530	232.9	17.09	†			
tEME-AE	$32_{5,28}$–$32_{4,29}$	213 676.802	232.9	17.06	†			
tEME-EA	$32_{5,28}$–$32_{4,29}$	213 679.692	232.9	17.13	213 680.0	0.14	0.03	CH_3COOCH_3
tEME-AA	$32_{5,28}$–$32_{4,29}$	213 680.076	232.9	17.14	†			
tEME-EE’	$31_{5,27}$–$31_{4,28}$	213 854.674	220.5	16.34	…	…	0.05	CH_3CH_2OH
tEME-EE	$31_{5,27}$–$31_{4,28}$	213 854.982	220.5	16.44	†			
tEME-AE	$31_{5,27}$–$31_{4,28}$	213 855.220	220.5	16.39	†			
tEME-EE	$28_{5,23}$–$28_{4,24}$	213 856.708	185.7	14.18	…	…	0.05	CH_3CH_2OH
tEME-AE	$28_{5,23}$–$28_{4,24}$	213 857.473	185.7	13.94	†			
tEME-EE’	$28_{5,23}$–$28_{4,24}$	213 857.509	185.7	13.70	†			
tEME-EA	$31_{5,27}$–$31_{4,28}$	213 858.239	220.5	16.52	…	…	0.05	CH_3CH_2OH
tEME-AA	$31_{5,27}$–$31_{4,28}$	213 858.632	220.5	16.53	†			
tEME-EA	$28_{5,23}$–$28_{4,24}$	213 859.015	185.7	14.70	†			
tEME-AA	$28_{5,23}$–$28_{4,24}$	213 859.367	185.7	14.73	†			
tEME-EE’	$30_{5,26}$–$30_{4,27}$	214 028.729	208.6	15.59	…	…	0.05	CH_3COCH_3
tEME-EE	$30_{5,26}$–$30_{4,27}$	214 029.157	208.6	15.76	†			
tEME-AE	$30_{5,26}$–$30_{4,27}$	214 029.345	208.6	15.68	†			
tEME-EA	$30_{5,26}$–$30_{4,27}$	214 032.539	208.6	15.91	…	…	0.04	

Species	Transition $J_{K_a,K_c} - J'_{K'_a,K'_c}$	Predicted frequency (MHz)	E_{upp} (K)	S_{ij}	Observed[1] frequency (MHz)	Observed[1] T_{MB} (K)	Model[2] T_{MB} (K)	Blends
tEME-AA	$30_{5,26}$–$30_{4,27}$	214 032.943	208.6	15.92	†			
tEME-EE	$27_{5,22}$–$27_{4,23}$	214 131.118	174.9	13.15	…	…	0.04	$CH_3CH_2{}^{13}CN$, CH_3COOH $v_t = 1$
tEME-AE	$27_{5,22}$–$27_{4,23}$	214 132.010	174.9	12.80	†			
tEME-EE’	$27_{5,22}$–$27_{4,23}$	214 132.166	174.9	12.45	†			
tEME-EA	$27_{5,22}$–$27_{4,23}$	214 133.150	174.9	14.07	…	…	0.04	$CH_3CH_2{}^{13}CN$, CH_3COOH $v_t = 1$
tEME-AA	$27_{5,22}$–$27_{4,23}$	214 133.486	174.9	14.14	†			
tEME-EE’	$29_{5,25}$–$29_{4,25}$	214 196.531	196.9	14.72	…	…	0.05	$CH_3{}^{13}CH_2CN$, $CH_3O^{13}COH$ $v_t = 1$
tEME-EE	$29_{5,25}$–$29_{4,25}$	214 197.122	196.9	15.02	†			
tEME-AE	$29_{5,25}$–$29_{4,25}$	214 197.239	196.9	14.88	†			
tEME-EA	$29_{5,25}$–$29_{4,25}$	214 200.673	196.9	15.30	…	…	0.04	$CH_3{}^{13}CH_2CN$, $CH_3O^{13}COH$ $v_t = 1$
tEME-AA	$29_{5,25}$–$29_{4,25}$	214 201.091	196.9	15.32	†			
tEME-EE’	$21_{2,20}$–$20_{1,19}$	214 246.202	93.7	7.76	214 246.2	0.15	0.09	$^{13}CH_3CN$
tEME-EE	$21_{2,20}$–$20_{1,19}$	214 246.202	93.7	7.76	†			
tEME-AE	$21_{2,20}$–$20_{1,19}$	214 246.332	93.7	7.76	†			
tEME-EA	$21_{2,20}$–$20_{1,19}$	214 247.602	93.7	7.76	214 247.7	0.11	0.06	$^{13}CH_3CN$
tEME-AA	$21_{2,20}$–$20_{1,19}$	214 247.732	93.7	7.76	†			
tEME-EE’	$26_{5,22}$–$26_{4,22}$	214 355.828	164.4	2.47	…	…	0.05	SO, $^{13}CH_3CN$
tEME-EE’	$28_{5,24}$–$28_{4,25}$	214 356.510	185.7	13.69	†			
tEME-AE	$26_{5,22}$–$26_{4,22}$	214 356.963	164.4	2.08	†			
tEME-EE	$26_{5,22}$–$26_{4,22}$	214 357.232	164.4	1.63	†			
tEME-EE	$28_{5,24}$–$28_{4,25}$	214 357.312	185.7	14.17	†			
tEME-AE	$28_{5,24}$–$28_{4,25}$	214 357.333	185.7	13.93	†			
tEME-EA	$28_{5,24}$–$28_{4,25}$	214 361.091	185.7	14.69	…	…	0.04	SO, $^{13}CH_3CN$
tEME-AA	$28_{5,24}$–$28_{4,25}$	214 361.527	185.7	14.72	†			
tEME-EE	$26_{5,21}$–$26_{4,22}$	214 369.161	164.4	11.92	…	…	0.07	SO, $^{13}CH_3CN$
tEME-AE	$26_{5,21}$–$26_{4,22}$	214 370.185	164.4	11.47	†			
tEME-EE’	$26_{5,21}$–$26_{4,22}$	214 370.456	164.4	11.08	†			
tEME-EA	$26_{5,21}$–$26_{4,22}$	214 370.843	164.4	13.42	†			
tEME-AA	$26_{5,21}$–$26_{4,22}$	214 371.154	164.4	13.55	†			
tEME-EE’	$27_{5,23}$–$27_{4,24}$	214 507.462	174.9	12.45	…	…	0.04	CH_3CH_2CN
tEME-AE	$27_{5,23}$–$27_{4,24}$	214 508.414	174.9	12.79	†			
tEME-EE	$27_{5,23}$–$27_{4,24}$	214 508.510	174.9	13.15	†			
tEME-EA	$27_{5,23}$–$27_{4,24}$	214 512.591	174.9	14.07	…	…	0.04	CH_3CH_2CN
tEME-AA	$27_{5,23}$–$27_{4,24}$	214 513.051	174.9	14.13	†			
tEME-EE	$25_{5,20}$–$25_{4,21}$	214 575.213	154.4	10.55	…	…	0.09	$^{13}C^{17}O$
tEME-AE	$25_{5,20}$–$25_{4,21}$	214 576.349	154.4	10.10	†			
tEME-EA	$25_{5,20}$–$25_{4,21}$	214 576.498	154.4	12.69	†			
tEME-EE’	$25_{5,20}$–$25_{4,21}$	214 576.706	154.4	9.74	†			
tEME-AA	$25_{5,20}$–$25_{4,21}$	214 576.769	154.4	12.96	†			

Species	Transition $J_{K_a,K_c} - J'_{K'_a,K'_c}$	Predicted frequency (MHz)	E_{upp} (K)	S_{ij}	Observed[1] frequency (MHz)	Observed[1] T_{MB} (K)	Model[2] T_{MB} (K)	Blends
tEME-EE'	$26_{5,22}$–$26_{4,23}$	214 648.535	164.4	11.08	…	…	0.04	CH_3OCOH
tEME-AE	$26_{5,22}$–$26_{4,23}$	214 649.611	164.4	11.47	†			
tEME-EE	$26_{5,22}$–$26_{4,23}$	214 649.829	164.4	11.92	†			
tEME-EA	$26_{5,22}$–$26_{4,23}$	214 654.288	164.5	13.41	…	…	0.04	CH_3OCOH
tEME-AA	$26_{5,22}$–$26_{4,23}$	214 654.781	164.5	13.54	†			
tEME-EE	$24_{5,19}$–$24_{4,20}$	214 753.118	144.7	9.23	214 754.3	0.20	0.09	
tEME-EA	$24_{5,19}$–$24_{4,20}$	214 754.023	144.7	11.84	†			
tEME-AA	$24_{5,19}$–$24_{4,20}$	214 754.233	144.7	12.38	†			
tEME-AE	$24_{5,19}$–$24_{4,20}$	214 754.329	144.7	8.86	†			
tEME-EE'	$24_{5,19}$–$24_{4,20}$	214 754.733	144.7	8.60	†			
tEME-EE'	$25_{5,21}$–$25_{4,22}$	214 779.208	154.4	9.74	…	…	0.04	CH_3OCOH
tEME-AE	$25_{5,21}$–$25_{4,22}$	214 780.378	154.4	10.10	†			
tEME-EE	$25_{5,21}$–$25_{4,22}$	214 780.701	154.4	10.55	†			
tEME-EA	$25_{5,21}$–$25_{4,22}$	214 785.581	154.4	12.69	…	…	0.04	CH_3OCOH
tEME-AA	$25_{5,21}$–$25_{4,22}$	214 786.123	154.4	12.96	†			
tEME-EE'	$24_{5,20}$–$24_{4,21}$	214 899.228	144.7	8.61	…	…	0.04	CH_3OCOH $v_t = 1$
tEME-AE	$24_{5,20}$–$24_{4,21}$	214 900.454	144.7	8.87	†			
tEME-EE	$24_{5,20}$–$24_{4,21}$	214 900.844	144.7	9.23	†			
tEME-EA	$24_{5,20}$–$24_{4,21}$	214 906.128	144.7	11.83	…	…	0.11	CH_3CH_2CN
tEME-EE	$23_{5,18}$–$23_{4,19}$	214 906.260	135.4	8.13	†			
tEME-AA	$24_{5,20}$–$24_{4,21}$	214 906.739	144.7	12.38	†			
tEME-EA	$23_{5,18}$–$23_{4,19}$	214 906.872	135.4	10.76	†			
tEME-AA	$23_{5,18}$–$23_{4,19}$	214 906.992	135.4	11.80	†			
tEME-AE	$23_{5,18}$–$23_{4,19}$	214 907.507	135.4	7.91	†			
tEME-EE'	$23_{5,18}$–$23_{4,19}$	214 907.924	135.4	7.77	†			
tEME-EE	$24_{5,19}$–$24_{4,21}$	214 909.858	144.7	3.15	†			
tEME-EA	$24_{5,19}$–$24_{4,21}$	214 910.548	144.7	0.55	†			
tEME-AE	$24_{5,19}$–$24_{4,21}$	214 911.166	144.7	3.51	†			
tEME-EE'	$24_{5,19}$–$24_{4,21}$	214 911.685	144.7	3.77	†			
tEME-EE'	$23_{5,19}$–$23_{4,20}$	215 008.545	135.4	7.77	…	…	0.02	CH_3CH_2CN v_{13}/v_{21}
tEME-AE	$23_{5,19}$–$23_{4,20}$	215 009.791	135.4	7.91	…	…	0.04	CH_3CH_2CN v_{13}/v_{21}
tEME-EE	$23_{5,19}$–$23_{4,20}$	215 010.209	135.4	8.13	†			
tEME-EA	$23_{5,19}$–$23_{4,20}$	215 015.810	135.4	10.75	215 016.7	0.05	0.04	
tEME-AA	$23_{5,19}$–$23_{4,20}$	215 016.519	135.4	11.80	†			
tEME-EA	$22_{5,18}$–$22_{4,18}$	215 035.544	126.6	1.78	…	…	0.07	CH_3CH_2CN
tEME-EE	$22_{5,17}$–$22_{4,18}$	215 037.639	126.6	7.33	†			
tEME-EA	$22_{5,17}$–$22_{4,18}$	215 038.085	126.6	9.45	†			
tEME-AA	$22_{5,17}$–$22_{4,18}$	215 038.089	126.6	11.23	†			
tEME-AE	$22_{5,17}$–$22_{4,18}$	215 038.890	126.6	7.24	†			
tEME-EE'	$22_{5,17}$–$22_{4,18}$	215 039.292	126.6	7.21	†			
tEME-AA	$35_{2,33}$–$34_{3,32}$	215 107.148	250.8	9.27	…	…	0.03	CH_3CH_2CN

Species	Transition $J_{K_a,K_c} - J'_{K'_a,K'_c}$	Predicted frequency (MHz)	E_{upp} (K)	S_{ij}	Observed[1] frequency (MHz)	Observed[1] T_{MB} (K)	Model[2] T_{MB} (K)	Blends
tEME-EA	$35_{2,33}–34_{3,32}$	215 107.270	250.8	9.27	†			
tEME-EE'	$22_{5,18}–22_{4,19}$	215 107.270	126.6	7.21	†			
tEME-AE	$22_{5,18}–22_{4,19}$	215 108.508	126.6	7.24	†			
tEME-EE	$22_{5,18}–22_{4,19}$	215 108.923	126.6	7.33	…	…	0.05	CH_3CH_2CN
tEME-AE	$35_{2,33}–34_{3,32}$	215 109.184	250.8	9.27	†			
tEME-EE	$35_{2,33}–34_{3,32}$	215 109.306	250.8	9.27	†			
tEME-EE'	$35_{2,33}–34_{3,32}$	215 109.306	250.8	9.27	†			
tEME-EA	$22_{5,18}–22_{4,19}$	215 114.713	126.6	9.45	…	…	0.04	CH_3CH_2CN
tEME-AA	$22_{5,18}–22_{4,19}$	215 115.545	126.6	11.23	†			
tEME-EE	$22_{5,17}–22_{4,19}$	215 117.232	126.6	3.90	†			
tEME-EA	$22_{5,17}–22_{4,19}$	215 117.254	126.6	1.78	†			
tEME-AE	$22_{5,17}–22_{4,19}$	215 118.679	126.6	3.99	†			
tEME-EE'	$22_{5,17}–22_{4,19}$	215 119.312	126.6	4.02	†			
tEME-EA	$21_{5,17}–21_{4,17}$	215 148.139	118.0	2.58	215 150.3	0.25	0.07	CH_3COCH_3
tEME-EE	$21_{5,16}–21_{4,17}$	215 149.914	118.0	6.81	†			
tEME-AA	$21_{5,16}–21_{4,17}$	215 150.202	118.0	10.66	†			
tEME-EA	$21_{5,16}–21_{4,17}$	215 150.327	118.0	8.07	†			
tEME-AE	$21_{5,16}–21_{4,17}$	215 151.142	118.0	6.84	†			
tEME-EE'	$21_{5,16}–21_{4,17}$	215 151.503	118.0	6.91	†			
tEME-EE'	$21_{5,17}–21_{4,18}$	215 195.665	118.0	6.91	…	…	0.04	SO
tEME-AE	$21_{5,17}–21_{4,18}$	215 196.869	118.0	6.84	†			
tEME-EE	$21_{5,17}–21_{4,18}$	215 197.254	118.0	6.81	†			
tEME-EA	$21_{5,17}–21_{4,18}$	215 203.100	118.0	8.07	…	…	0.04	SO
tEME-AA	$21_{5,17}–21_{4,18}$	215 204.068	118.0	10.66	†			
tEME-EA	$21_{5,16}–21_{4,18}$	215 205.287	118.0	2.58	†			
tEME-EE	$21_{5,16}–21_{4,18}$	215 205.486	118.0	3.85	†			
tEME-EA	$20_{5,16}–20_{4,16}$	215 243.901	109.9	3.19	…	…	0.07	SO
tEME-EE	$20_{5,15}–20_{4,16}$	215 245.438	109.9	6.54	†			
tEME-AA	$20_{5,15}–20_{4,16}$	215 245.691	109.9	10.09	†			
tEME-EA	$20_{5,15}–20_{4,16}$	215 245.934	109.9	6.89	†			
tEME-AE	$20_{5,15}–20_{4,16}$	215 246.615	109.9	6.68	†			
tEME-EE'	$20_{5,15}–20_{4,16}$	215 246.907	109.9	6.83	†			
tEME-EE'	$20_{5,16}–20_{4,17}$	215 274.126	109.9	6.83	…	…	0.04	CH_3CH_2CN v_{20} = 1
tEME-AE	$20_{5,16}–20_{4,17}$	215 275.268	109.9	6.68	†			
tEME-EE	$20_{5,16}–20_{4,17}$	215 275.595	109.9	6.54	†			
tEME-EA	$20_{5,16}–20_{4,17}$	215 281.378	109.9	6.89	…	…	0.04	CH_3CH_2CN v_{13}/v_{21}
tEME-AA	$20_{5,16}–20_{4,17}$	215 282.470	109.9	10.09	†			
tEME-EA	$20_{5,15}–20_{4,17}$	215 283.411	109.9	3.19	†			
tEME-EE	$20_{5,15}–20_{4,17}$	215 283.810	109.9	3.55	†			
tEME-EA	$19_{5,15}–19_{4,15}$	215 324.992	102.2	3.49	215 326.9	0.20	0.08	CH_3OCOH
tEME-EE	$19_{5,14}–19_{4,15}$	215 326.280	102.2	6.50	†			

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Species	Transition $J_{K_a,K_c} - J'_{K'_a,K'_c}$	Predicted frequency (MHz)	E_{upp} (K)	S_{ij}	Observed[1] frequency (MHz)	Observed[1] T_{MB} (K)	Model[2] T_{MB} (K)	Blends
tEME-AA	$19_{5,14}$–$19_{4,15}$	215 326.637	102.2	9.52	†			
tEME-EA	$19_{5,14}$–$19_{4,15}$	215 326.971	102.2	6.03	†			
tEME-AE	$19_{5,14}$–$19_{4,15}$	215 327.373	102.2	6.72	†			
tEME-EE’	$19_{5,14}$–$19_{4,15}$	215 327.561	102.2	6.95	†			
tEME-EE’	$19_{5,15}$–$19_{4,16}$	215 343.169	102.2	6.95	215 344.3	0.20	0.05	CH_3OCOH $v_t = 1$
tEME-AE	$19_{5,15}$–$19_{4,16}$	215 344.214	102.2	6.72	†			
tEME-EE	$19_{5,15}$–$19_{4,16}$	215 344.450	102.2	6.50	†			
tEME-EA	$19_{5,15}$–$19_{4,16}$	215 350.059	102.2	6.03	…	…	0.05	CH_3CH_2CN
tEME-AA	$19_{5,15}$–$19_{4,16}$	215 351.248	102.2	9.52	†			
tEME-EE’	$12_{3,10}$–$11_{2,9}$	215 361.252	40.5	4.16	…	…	0.07	CH_3CH_2CN v_{13}/v_{21}
tEME-EE	$12_{3,10}$–$11_{2,9}$	215 361.484	40.5	4.18	†			
tEME-AE	$12_{3,10}$–$11_{2,9}$	215 361.676	40.5	4.17	†			
tEME-EA	$12_{3,10}$–$11_{2,9}$	215 364.224	40.5	4.19	…	…	0.05	CH_3CH_2CN v_{13}/v_{21}
tEME-AA	$12_{3,10}$–$11_{2,9}$	215 364.533	40.5	4.20	†			
tEME-EE	$18_{5,13}$–$18_{4,14}$	215 394.256	94.8	6.65	…	…	0.11	CH_3CH_2CN
tEME-AA	$18_{5,13}$–$18_{4,14}$	215 394.875	94.8	8.95	†			
tEME-AE	$18_{5,13}$–$18_{4,14}$	215 395.227	94.8	6.94	†			
tEME-EA	$18_{5,13}$–$18_{4,14}$	215 395.264	94.8	5.47	†			
tEME-EE’	$18_{5,13}$–$18_{4,14}$	215 395.280	94.8	7.19	†			
tEME-EE’	$18_{5,14}$–$18_{4,15}$	215 403.394	94.8	7.19	…	…	0.06	CH_3CH_2CN
tEME-AE	$18_{5,14}$–$18_{4,15}$	215 404.308	94.8	6.94	†			
tEME-EE	$18_{5,14}$–$18_{4,15}$	215 404.417	94.8	6.65	†			
tEME-EA	$18_{5,14}$–$18_{4,15}$	215 409.728	94.8	5.47	…	…	0.09	CH_3CH_2CN $v = 0$; v_{13}/v_{21}
tEME-AA	$18_{5,14}$–$18_{4,15}$	215 410.979	94.8	8.95	†			
tEME-EA	$17_{5,13}$–$17_{4,13}$	215 450.467	87.9	3.22	215 451.8	0.47	0.11	CH_3CH_2CN $v_{20} = 1$, NH_2CHO $v_{12} = 1$
tEME-EE	$17_{5,13}$–$17_{4,13}$	215 450.974	87.9	6.90	†			
tEME-EE’	$17_{5,13}$–$17_{4,13}$	215 451.703	87.9	7.39	†			
tEME-AE	$17_{5,13}$–$17_{4,13}$	215 451.799	87.9	7.18	†			
tEME-AA	$17_{5,13}$–$17_{4,13}$	215 452.025	87.9	8.39	†			
tEME-EA	$17_{5,13}$–$17_{4,13}$	215 452.436	87.9	5.17	†			
tEME-EE’	$17_{5,13}$–$17_{4,13}$	215 455.422	87.9	7.39	…	…	0.07	CH_3CH_2CN v_{13}/v_{21}, CH_3CH_2OH
tEME-EE	$17_{5,13}$–$17_{4,13}$	215 456.151	87.9	6.90	†			
tEME-AE	$17_{5,13}$–$17_{4,13}$	215 456.193	87.9	7.18	†			
tEME-EA	$17_{5,13}$–$17_{4,14}$	215 461.025	87.9	5.17	…	…	0.04	CH_3CH_2CN v_{13}/v_{21}, CH_3CH_2OH
tEME-AA	$17_{5,13}$–$17_{4,14}$	215 462.304	87.9	8.39	†			
tEME-EA	$17_{5,12}$–$17_{4,14}$	215 462.994	87.9	3.22	†			
tEME-EE’	$27_{1,27}$–$26_{0,26}$	215 478.840	144.2	21.60	…	…	0.24	CH_3CH_2CN v_{13}/v_{21}
tEME-EE	$27_{1,27}$–$26_{0,26}$	215 478.840	144.2	21.60	†			
tEME-AE	$27_{1,27}$–$26_{0,26}$	215 478.854	144.2	21.60	†			
tEME-EA	$27_{1,27}$–$26_{0,26}$	215 479.025	144.2	21.60	†			
tEME-AA	$27_{1,27}$–$26_{0,26}$	215 479.039	144.2	21.60	†			

Species	Transition $J_{K_a,K_c} - J'_{K'_a,K'_c}$	Predicted frequency (MHz)	E_{upp} (K)	S_{ij}	Observed[1] frequency (MHz)	Observed[1] T_{MB} (K)	Model[2] T_{MB} (K)	Blends
tEME-EE	$16_{5,11}$–$16_{4,12}$	215 497.897	81.3	7.05	…	…	0.09	CH_3OCH_3, CH_3CH_2CN v_{13}/v_{21}
tEME-EA	$16_{5,12}$–$16_{4,12}$	215 497.943	81.3	2.74	†			
tEME-EE’	$16_{5,11}$–$16_{4,12}$	215 498.372	81.3	7.37	†			
tEME-AE	$16_{5,11}$–$16_{4,12}$	215 498.590	81.3	7.24	†			
tEME-AA	$16_{5,11}$–$16_{4,12}$	215 499.524	81.3	7.82	…	…	0.11	CH_3OCH_3, CH_3CH_2CN v_{13}/v_{21}
tEME-EE’	$16_{5,12}$–$16_{4,13}$	215 499.830	81.3	7.37	†			
tEME-EA	$16_{5,11}$–$16_{4,12}$	215 499.921	81.3	5.08	†			
tEME-EE	$16_{5,12}$–$16_{4,13}$	215 500.305	81.3	7.05	†			
tEME-AE	$16_{5,12}$–$16_{4,13}$	215 500.485	81.3	7.24	†			
tEME-EA	$16_{5,11}$–$16_{4,12}$	215 504.636	81.3	5.08	…	…	0.05	CH_3OCH_3, CH_3CH_2CN v_{13}/v_{21}, $^{33}SH_2$
tEME-AA	$16_{5,12}$–$16_{4,13}$	215 505.905	81.3	7.82	†			
tEME-EA	$16_{5,12}$–$16_{4,13}$	215 506.613	81.3	2.74	†			
tEME-EE	$15_{5,10}$–$15_{4,11}$	215 536.404	75.1	6.94	215 536.9	0.25	0.15	CH_3OCOH v_t = 1
tEME-EE’	$15_{5,10}$–$15_{4,11}$	215 536.720	75.1	7.08	†			
tEME-EA	$15_{5,11}$–$15_{4,11}$	215 537.002	75.1	2.05	†			
tEME-AE	$15_{5,10}$–$15_{4,11}$	215 537.010	75.1	7.03	†			
tEME-EE’	$15_{5,11}$–$15_{4,12}$	215 537.169	75.1	7.08	†			
tEME-EE	$15_{5,11}$–$15_{4,12}$	215 537.485	75.1	6.94	†			
tEME-AE	$15_{5,11}$–$15_{4,12}$	215 537.757	75.1	7.03	†			
tEME-AA	$15_{5,10}$–$15_{4,11}$	215 538.650	75.1	7.25	…	…	0.04	CH_3OCOH v_t = 1, CH_3CH_2CN v_{13}/v_{21}
tEME-EA	$15_{5,10}$–$15_{4,11}$	215 538.990	75.1	5.21	†			
tEME-AA	$15_{5,10}$–$15_{4,11}$	215 538.650	75.1	7.25	†			
tEME-EA	$15_{5,10}$–$15_{4,11}$	215 538.990	75.1	5.21	†			
tEME-EA	$15_{5,11}$–$15_{4,12}$	215 541.270	75.1	5.21	†			
tEME-AA	$15_{5,11}$–$15_{4,12}$	215 542.488	75.1	7.25	†			
tEME-EE	$14_{5,9}$–$14_{4,10}$	215 567.750	69.3	6.58	…	…	0.17	CH_3CH_2CN v_{20} = 1
tEME-EE’	$14_{5,9}$–$14_{4,10}$	215 567.993	69.3	6.63	†			
tEME-EE’	$14_{5,10}$–$14_{4,11}$	215 568.043	69.3	6.63	†			
tEME-EE	$14_{5,10}$–$14_{4,11}$	215 568.286	69.3	6.58	†			
tEME-AE	$14_{5,9}$–$14_{4,10}$	215 568.316	69.3	6.61	†			
tEME-AE	$14_{5,10}$–$14_{4,11}$	215 568.602	69.3	6.61	†			
tEME-EA	$14_{5,10}$–$14_{4,10}$	215 568.774	69.3	1.23	†			
tEME-AA	$14_{5,9}$–$14_{4,10}$	215 570.539	69.3	6.68	…	…	0.06	CH_3CH_2CN $v13/v21$
tEME-EA	$14_{5,9}$–$14_{4,10}$	215 570.772	69.3	5.45	†			
tEME-EA	$14_{5,10}$–$14_{4,11}$	215 571.650	69.3	5.45	†			
tEME-AA	$14_{5,10}$–$14_{4,11}$	215 572.766	69.3	6.68	…	…	0.04	CH_3CH_2CN v_{13}/v_{21}
tEME-EA	$14_{5,9}$–$14_{4,11}$	215 573.648	69.3	1.23	†			
tEME-EE	$13_{5,8}$–$13_{4,9}$	215 593.014	63.9	6.08	…	…	0.17	CH_3CH_2CN v_{20} = 1, SiO v = 1
tEME-EE’	$13_{5,9}$–$13_{4,10}$	215 593.138	63.9	6.09	†			

Species	Transition $J_{K_a,K_c} - J'_{K'_a,K'_c}$	Predicted frequency (MHz)	E_{upp} (K)	S_{ij}	Observed[1] frequency (MHz)	Observed[1] T_{MB} (K)	Model[2] T_{MB} (K)	Blends
tEME-EE’	$13_{5,8}–13_{4,9}$	215 593.228	63.9	6.09	†			
tEME-EE	$13_{5,9}–13_{4,10}$	215 593.353	63.9	6.08	†			
tEME-AE	$13_{5,8}–13_{4,9}$	215 593.566	63.9	6.09	†			
tEME-AE	$13_{5,9}–13_{4,10}$	215 593.687	63.9	6.09	†			
tEME-AA	$13_{5,8}–13_{4,9}$	215 596.207	63.9	6.11	…	…	0.09	$CH_3CH_2{}^{13}CN$, SiO v = 1
tEME-EA	$13_{5,8}–13_{4,9}$	215 596.289	63.9	5.58	†			
tEME-EA	$13_{5,9}–13_{4,10}$	215 596.478	63.9	5.58	†			
tEME-EE	$12_{5,7}–12_{4,8}$	215 613.102	58.9	5.52	…	…	0.18	CH_3CH_2OH, CH_3OCOH v_t = 1, CH_3CH_2CN
tEME-EE’	$12_{5,8}–12_{4,9}$	215 613.172	58.9	5.53	†			
tEME-EE’	$12_{5,7}–12_{4,8}$	215 613.308	58.9	5.53	†			
tEME-EE	$12_{5,8}–12_{4,9}$	215 613.378	58.9	5.52	†			
tEME-AE	$12_{5,7}–12_{4,8}$	215 613.651	58.9	5.52	†			
tEME-AE	$12_{5,8}–12_{4,9}$	215 613.720	58.9	5.52	†			
tEME-EA	$12_{5,8}–12_{4,9}$	215 616.405	58.9	5.37	…	…	0.10	CH_3CH_2CN
tEME-EA	$12_{5,7}–12_{4,8}$	215 616.490	58.9	5.37	†			
tEME-AA	$12_{5,7}–12_{4,8}$	215 616.564	58.9	5.53	†			
tEME-AA	$12_{5,8}–12_{4,9}$	215 617.221	58.9	5.53	†			
tEME-EE	$11_{5,6}–11_{4,7}$	215 628.800	54.3	4.94	…	…	0.16	CH_3CH_2CN
tEME-EE’	$11_{5,7}–11_{4,8}$	215 628.855	54.3	4.94	†			
tEME-EE’	$11_{5,6}–11_{4,7}$	215 629.003	54.3	4.94	†			
tEME-EE	$11_{5,7}–11_{4,8}$	215 629.058	54.3	4.94	†			
tEME-AE	$11_{5,6}–11_{4,7}$	215 629.349	54.3	4.94	†			
tEME-AE	$11_{5,7}–11_{4,8}$	215 629.404	54.3	4.94	…	…	0.10	CH_3CH_2CN
tEME-EA	$11_{5,7}–11_{4,8}$	215 632.056	54.3	4.91	†			
tEME-EA	$11_{5,6}–11_{4,7}$	215 632.229	54.3	4.91	†			
tEME-AA	$11_{5,6}–11_{4,7}$	215 632.425	54.3	4.94	†			
tEME-AA	$11_{5,7}–11_{4,8}$	215 632.754	54.3	4.94	†			
tEME-EE	$10_{5,5}–10_{4,6}$	215 640.803	50.0	4.35	215 641.1	0.18	0.13	CH_3COOH
tEME-EE’	$10_{5,6}–10_{4,7}$	215 640.854	50.0	4.35	†			
tEME-EE’	$10_{5,5}–10_{4,6}$	215 641.007	50.0	4.35	†			
tEME-EE	$10_{5,6}–10_{4,7}$	215 641.058	50.0	4.35	†			
tEME-AE	$10_{5,5}–10_{4,6}$	215 641.354	50.0	4.35	†			
tEME-AE	$10_{5,6}–10_{4,7}$	215 641.405	50.0	4.35	†			
tEME-EA	$10_{5,6}–10_{4,7}$	215 644.051	50.0	4.34	215 644.4	0.21	0.10	CH_3COOH
tEME-EA	$10_{5,5}–10_{4,6}$	215 644.248	50.0	4.34	†			
tEME-AA	$10_{5,5}–10_{4,6}$	215 644.522	50.0	4.35	†			
tEME-AA	$10_{5,6}–10_{4,7}$	215 644.676	50.0	4.35	†			
tEME-EE	$9_{5,4}–9_{4,5}$	215 649.740	46.1	3.73	215 650.1	0.42	0.12	CH_3CH_2CN v_{20} = 1
tEME-EE’	$9_{5,5}–9_{4,6}$	215 649.791	46.1	3.73	†			
tEME-EE’	$9_{5,4}–9_{4,5}$	215 649.944	46.1	3.73	†			

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Species	**Transition** $J_{K_a,K_c} - J'_{K'_a,K'_c}$	**Predicted frequency (MHz)**	E_{upp} **(K)**	S_{ij}	**Observed[1] frequency (MHz)**	**Observed[1]** T_{MB} **(K)**	**Model[2]** T_{MB} **(K)**	**Blends**
tEME-EE	$9_{5,5}$–$9_{4,6}$	215 649.995	46.1	3.73	†			
tEME-AE	$9_{5,4}$–$9_{4,5}$	215 650.292	46.1	3.73	†			
tEME-AE	$9_{5,5}$–$9_{4,6}$	215 650.343	46.1	3.73	†			
tEME-EA	$9_{5,5}$–$9_{4,6}$	215 652.990	46.1	3.73	215 653.4	0.42	0.08	CH_3CH_2CN v_{20} = 1
tEME-EA	$9_{5,4}$–$9_{4,5}$	215 653.193	46.1	3.73	†			
tEME-AA	$9_{5,4}$–$9_{4,5}$	215 653.509	46.1	3.73	†			
tEME-AA	$9_{5,5}$–$9_{4,6}$	215 653.575	46.1	3.73	†			
tEME-EE	$8_{5,3}$–$8_{4,4}$	215 656.176	42.7	3.10	215 656.4	0.43	0.11	CH_3CH_2CN v_{20} = 1
tEME-EE’	$8_{5,4}$–$8_{4,5}$	215 656.227	42.7	3.10	†			
tEME-EE’	$8_{5,3}$–$8_{4,4}$	215 656.380	42.7	3.10	†			
tEME-EE	$8_{5,4}$–$8_{4,5}$	215 656.432	42.7	3.10	†			
tEME-AE	$8_{5,3}$–$8_{4,4}$	215 656.730	42.7	3.10	†			
tEME-AE	$8_{5,4}$–$8_{4,5}$	215 656.781	42.7	3.10	†			
tEME-EA	$8_{5,4}$–$8_{4,5}$	215 659.431	42.7	3.10	215 659.8	0.36	0.09	CH_3CH_2CN v_{20} = 1
tEME-EA	$8_{5,3}$–$8_{4,4}$	215 659.635	42.7	3.10	†			
tEME-AA	$8_{5,3}$–$8_{4,4}$	215 659.972	42.7	3.10	†			
tEME-AA	$8_{5,4}$–$8_{4,5}$	215 659.998	42.7	3.10	†			
tEME-EE	$7_{5,2}$–$7_{4,3}$	215 660.620	39.6	2.43	215 660.8	0.34	0.11	CH_3CH_2CN v_{20} = 1
tEME-EE’	$7_{5,3}$–$7_{4,4}$	215 660.672	39.6	2.43	†			
tEME-EE’	$7_{5,2}$–$7_{4,3}$	215 660.825	39.6	2.43	†			
tEME-EE	$7_{5,3}$–$7_{4,4}$	215 660.877	39.6	2.43	†			
tEME-AE	$7_{5,2}$–$7_{4,3}$	215 661.175	39.6	2.43	†			
tEME-AE	$7_{5,3}$–$7_{4,4}$	215 661.227	39.6	2.43	†			
tEME-EE	$6_{5,1}$–$6_{4,2}$	215 663.523	36.9	1.72	215 663.9	0.30	0.11	CH_3CH_2CN v_{20} = 1
tEME-EE’	$6_{5,2}$–$6_{4,3}$	215 663.575	36.9	1.72	†			
tEME-EE’	$6_{5,1}$–$6_{4,2}$	215 663.728	36.9	1.72	†			
tEME-EE	$6_{5,2}$–$6_{4,3}$	215 663.780	36.9	1.72	†			
tEME-EA	$7_{5,3}$–$7_{4,4}$	215 663.879	39.6	2.43	†			
tEME-AE	$6_{5,1}$–$6_{4,2}$	215 664.080	36.9	1.72	†			
tEME-EA	$7_{5,2}$–$7_{4,3}$	215 664.084	39.6	2.43	†			
tEME-AE	$6_{5,2}$–$6_{4,3}$	215 664.131	36.9	1.72	†			
tEME-AA	$7_{5,2}$–$7_{4,3}$	215 664.430	39.6	2.43	†			
tEME-AA	$7_{5,3}$–$7_{4,4}$	215 664.439	39.6	2.43	†			
tEME-EE	$5_{5,0}$–$5_{4,1}$	215 665.279	34.6	0.92	†			
tEME-EE’	$5_{5,1}$–$5_{4,2}$	215 665.331	34.6	0.92	†			
tEME-EE’	$5_{5,0}$–$5_{4,1}$	215 665.485	34.6	0.92	†			
tEME-EE	$5_{5,1}$–$5_{4,2}$	215 665.537	34.6	0.92	†			
tEME-AE	$5_{5,0}$–$5_{4,1}$	215 665.837	34.6	0.92	†			
tEME-AE	$5_{5,1}$–$5_{4,2}$	215 665.889	34.6	0.92	†			
tEME-EA	$6_{5,2}$–$6_{4,2}$	215 666.786	36.9	1.72	…	…	0.05	CH_3CH_2CN v = 0, v_{20} = 1
tEME-EA	$6_{5,1}$–$6_{4,2}$	215 666.991	36.9	1.72	†			

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Species	Transition $J_{K_a,K_c} - J'_{K'_a,K'_c}$	Predicted frequency (MHz)	E_{upp} (K)	S_{ij}	Observed frequency (MHz)[1]	Observed T_{MB} (K)[1]	Model T_{MB} (K)[2]	Blends
tEME-EA	$5_{5,1}$–$5_{4,2}$	215 668.545	34.6	0.92	†			
tEME-EA	$5_{5,0}$–$5_{4,1}$	215 668.751	34.6	0.92	†			
tEME-AA	$5_{5,0}$–$5_{4,1}$	215 669.103	34.6	0.92	†			
tEME-AA	$5_{5,1}$–$5_{4,2}$	215 669.103	34.6	0.92	†			
tEME-EE'	$6_{4,3}$–$5_{3,3}$	216 054.535	26.5	3.73	216 054.9	0.30	0.08	CH_3CH_2CN v_{13}/v_{21}
tEME-EE	$6_{4,3}$–$5_{3,3}$	216 054.868	26.5	3.73	†			
tEME-AE	$6_{4,3}$–$5_{3,3}$	216 055.095	26.5	3.73	†			
tEME-EE	$6_{4,2}$–$5_{3,2}$	216 055.759	26.5	3.73	†			
tEME-EE'	$6_{4,2}$–$5_{3,2}$	216 056.093	26.5	3.73	216 056.4	0.26	0.08	CH_3CH_2CN v_{13}/v_{21}
tEME-AE	$6_{4,2}$–$5_{3,2}$	216 056.319	26.5	3.73	†			
tEME-EA	$6_{4,3}$–$5_{3,3}$	216 058.222	26.5	3.69	216 058.4	0.25	0.10	CH_3CH_2CN v_{13}/v_{21}
tEME-EA	$6_{4,2}$–$5_{3,2}$	216 058.519	26.5	3.69	†			
tEME-AA	$6_{4,3}$–$5_{3,2}$	216 058.597	26.5	3.73	†			
tEME-AA	$6_{4,2}$–$5_{3,3}$	216 058.930	26.5	3.73	†			
tEME-EE	$12_{3,9}$–$11_{2,10}$	217 007.530	40.5	4.14	217 007.7	0.13	0.08	HDCS, CH_3OCOH
tEME-EE'	$12_{3,9}$–$11_{2,10}$	217 007.763	40.5	4.12	†			
tEME-AE	$12_{3,9}$–$11_{2,10}$	217 007.939	40.5	4.13	†			
tEME-EA	$12_{3,9}$–$11_{2,10}$	217 009.762	40.5	4.16	217 010.0	0.13	0.05	HDCS, CH_3OCOH
tEME-AA	$12_{3,9}$–$11_{2,10}$	217 010.054	40.5	4.16	†			
tEME-AA	$30_{1,29}$–$29_{2,28}$	217 164.465	182.5	13.55	…	…	0.07	CH_3OCOH
tEME-EA	$30_{1,29}$–$29_{2,28}$	217 164.508	182.5	13.55	†			
tEME-AE	$30_{1,29}$–$29_{2,28}$	217 165.360	182.5	13.55	†			
tEME-EE	$30_{1,29}$–$29_{2,28}$	217 165.402	182.5	13.55	†			
tEME-EE'	$30_{1,29}$–$29_{2,28}$	217 165.402	182.5	13.55	†			
tEME-AA	$28_{0,28}$–$27_{1,27}$	217 940.650	154.7	22.59	217 940.7	0.44	0.25	c-C_3H_2, $HCC^{13}CN$ v_7 = 1,CH_3COOCH_3
tEME-EA	$28_{0,28}$–$27_{1,27}$	217 940.651	154.7	22.59	†			
tEME-AE	$28_{0,28}$–$27_{1,27}$	217 940.758	154.7	22.59	†			
tEME-EE	$28_{0,28}$–$27_{1,27}$	217 940.759	154.7	22.59	†			
tEME-EE'	$28_{0,28}$–$27_{1,27}$	217 940.759	154.7	22.59	†			
tEME-EE'	$22_{2,21}$–$21_{1,20}$	219 893.140	102.2	8.31	…	…	0.09	SO
tEME-EE	$22_{2,21}$–$21_{1,20}$	219 893.140	102.2	8.31	†			
tEME-AE	$22_{2,21}$–$21_{1,20}$	219 893.263	102.2	8.31	†			
tEME-EA	$22_{2,21}$–$21_{1,20}$	219 894.511	102.2	8.31	…	…	0.06	SO
tEME-AA	$22_{2,21}$–$21_{1,20}$	219 894.635	102.2	8.31	†			
tEME-EE'	$28_{1,28}$–$27_{0,27}$	222 861.487	154.8	22.63	222 861.3	0.55	0.26	CH_3OCOH
tEME-EE	$28_{1,28}$–$27_{0,27}$	222 861.487	154.8	22.63	†			
tEME-AE	$28_{1,28}$–$27_{0,27}$	222 861.500	154.8	22.63	†			
tEME-EA	$28_{1,28}$–$27_{0,27}$	222 861.655	154.8	22.63	†			
tEME-AA	$28_{1,28}$–$27_{0,27}$	222 861.668	154.8	22.63	†			
tEME-EE'	$13_{3,11}$–$12_{2,10}$	222 980.574	45.5	4.38	222 980.7	0.22	0.09	$CH_3O^{13}COH$
tEME-EE	$13_{3,11}$–$12_{2,10}$	222 980.720	45.5	4.39	†			

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Species	Transition $J_{K_a,K_c} - J'_{K'_a,K'_c}$	Predicted frequency (MHz)	E_{upp} (K)	S_{ij}	Observed[1] frequency (MHz)	Observed[1] T_{MB} (K)	Model[2] T_{MB} (K)	Blends
tEME-AE	$13_{3,11}$–$12_{2,10}$	222 980.951	45.5	4.39	†			
tEME-EA	$13_{3,11}$–$12_{2,10}$	222 983.368	45.5	4.40	222 983.7	0.16	0.06	$CH_3O^{13}COH$
tEME-AA	$13_{3,11}$–$12_{2,10}$	222 983.672	45.5	4.40	†			
tEME-EE	$16_{2,14}$–$15_{1,15}$	223 403.761	57.4	2.48	…	…	0.04	CH_3OCH_3, CH_3OCOH v_t = 1
tEME-EE’	$16_{2,14}$–$15_{1,15}$	223 403.762	57.4	2.48	†			
tEME-AE	$16_{2,14}$–$15_{1,15}$	223 404.001	57.4	2.48	†			
tEME-EA	$16_{2,14}$–$15_{1,15}$	223 405.432	57.4	2.48	…	…	0.03	CH_3OCH_3
tEME-AA	$16_{2,14}$–$15_{1,15}$	223 405.671	57.4	2.48	†			
tEME-EE’	$7_{4,4}$–$6_{3,4}$	224 103.753	29.2	3.89	224 103.98	0.63	0.10	CH_3CH_2CN v_{13}/v_{21}
tEME-EE	$7_{4,4}$–$6_{3,4}$	224 104.093	29.2	3.88	†			
tEME-AE	$7_{4,4}$–$6_{3,4}$	224 104.315	29.2	3.89	†			
tEME-EE	$7_{4,3}$–$6_{3,3}$	224 104.926	29.2	3.88	†			
tEME-EE’	$7_{4,3}$–$6_{3,3}$	224 105.266	29.2	3.89	224 105.2	0.47	0.10	CH_3CH_2CN v_{20} = 1
tEME-AE	$7_{4,3}$–$6_{3,3}$	224 105.490	29.2	3.89	†			
tEME-AA	$7_{4,4}$–$6_{3,3}$	224 107.456	29.2	3.90	224 107.7	0.52	0.10	CH_3CH_2CN v_{20} = 1
tEME-EA	$7_{4,4}$–$6_{3,4}$	224 107.546	29.2	3.58	†			
tEME-EA	$7_{4,3}$–$6_{3,3}$	224 107.581	29.2	3.58	†			
tEME-AA	$7_{4,3}$–$6_{3,4}$	224 108.457	29.2	3.90	†			
tEME-EE	$13_{3,10}$–$12_{2,11}$	225 283.674	45.5	4.33	…	…	0.09	CH_3CH_2OH
tEME-EE’	$13_{3,10}$–$12_{2,11}$	225 283.820	45.5	4.33	†			
tEME-AE	$13_{3,10}$–$12_{2,11}$	225 284.043	45.5	4.33	†			
tEME-EA	$13_{3,10}$–$12_{2,11}$	225 285.990	45.5	4.34	225 286.28	0.29	0.06	CH_3CH_2OH
tEME-AA	$13_{3,10}$–$12_{2,11}$	225 286.286	45.5	4.34	†			
tEME-EE’	$23_{2,22}$–$22_{1,21}$	225 494.508	111.0	8.90	225 494.4	0.12	0.10	
tEME-EE	$23_{2,22}$–$22_{1,21}$	225 494.508	111.0	8.90	†			
tEME-AE	$23_{2,22}$–$22_{1,21}$	225 494.625	111.0	8.90	†			
tEME-EA	$23_{2,22}$–$22_{1,21}$	225 495.848	111.0	8.90	225 495.9	0.12	0.07	
tEME-AA	$23_{2,22}$–$22_{1,21}$	225 495.965	111.0	8.90	†			
tEME-EA	$29_{0,29}$–$28_{1,28}$	226 057.836	165.7	23.62	226 057.9	0.65	0.26	CH_3CH_2OH
tEME-AA	$29_{0,29}$–$28_{1,28}$	226 057.836	165.7	23.62	†			
tEME-EE	$29_{0,29}$–$28_{1,28}$	226 057.928	165.7	23.62	†			
tEME-EE’	$29_{0,29}$–$28_{1,28}$	226 057.928	165.7	23.62	†			
tEME-AE	$29_{0,29}$–$28_{1,28}$	226 057.928	165.7	23.62	†			
tEME-AA	$31_{1,30}$–$30_{2,29}$	227 090.552	194.5	14.51	…	…	0.09	CH_3OH
tEME-EA	$31_{1,30}$–$30_{2,29}$	227 090.589	194.5	14.51	†			
tEME-AE	$31_{1,30}$–$30_{2,29}$	227 091.390	194.5	14.51	†			
tEME-EE	$31_{1,30}$–$30_{2,29}$	227 091.426	194.5	14.51	†			
tEME-EE’	$31_{1,30}$–$30_{2,29}$	227 091.426	194.5	14.51	†			
tEME-EE’	$29_{1,29}$–$28_{0,28}$	230 291.194	165.8	23.66	…	…	0.27	CH_3OH
tEME-EE	$29_{1,29}$–$28_{0,28}$	230 291.194	165.8	23.66	†			
tEME-AE	$29_{1,29}$–$28_{0,28}$	230 291.205	165.8	23.66	†			

Species	Transition $J_{K_a,K_c} - J'_{K'_a,K'_c}$	Predicted frequency (MHz)	E_{upp} (K)	S_{ij}	Observed[1] frequency (MHz)	Observed[1] T_{MB} (K)	Model[2] T_{MB} (K)	Blends
tEME-EA	$29_{1,29}$–$28_{0,28}$	230 291.345	165.8	23.66	†			
tEME-AA	$29_{1,29}$–$28_{0,28}$	230 291.357	165.8	23.66	†			
tEME-EE’	$14_{3,12}$–$13_{2,11}$	230 486.881	50.9	4.59	…	…	0.09	CO
tEME-EE	$14_{3,12}$–$13_{2,11}$	230 486.975	50.9	4.60	†			
tEME-AE	$14_{3,12}$–$13_{2,11}$	230 487.227	50.9	4.59	†			
tEME-EA	$14_{3,12}$–$13_{2,11}$	230 489.569	50.9	4.60	…	…	0.07	CO
tEME-AA	$14_{3,12}$–$13_{2,11}$	230 489.869	50.9	4.60	†			
tEME-EE’	$24_{2,23}$–$23_{1,22}$	231 063.540	120.2	9.52	…	…	0.11	OCS
tEME-EE	$24_{2,23}$–$23_{1,22}$	231 063.540	120.2	9.52	†			
tEME-AE	$24_{2,23}$–$23_{1,22}$	231 063.652	120.2	9.52	†			
tEME-EA	$24_{2,23}$–$23_{1,22}$	231 064.846	120.2	9.52	…	…	0.08	OCS
tEME-AA	$24_{2,23}$–$23_{1,22}$	231 064.958	120.2	9.52	†			
tEME-EE’	$8_{4,5}$–$7_{3,5}$	232 151.207	32.3	4.03	232 152.1	0.47	0.11	$^{13}CH_3CN$,CH_3OCOH v_t =1
tEME-EE	$8_{4,5}$–$7_{3,5}$	232 151.590	32.3	3.98	†			
tEME-AE	$8_{4,5}$–$7_{3,5}$	232 151.787	32.3	4.01	†			
tEME-EE	$8_{4,4}$–$7_{3,4}$	232 152.098	32.3	3.98	†			
tEME-EE’	$8_{4,4}$–$7_{3,4}$	232 152.480	32.3	4.03	†			
tEME-EA	$8_{4,5}$–$7_{3,4}$	232 152.521	32.3	1.00	†			
tEME-AE	$8_{4,4}$–$7_{3,4}$	232 152.685	32.3	4.01	†			
tEME-AA	$8_{4,5}$–$7_{3,4}$	232 154.033	32.3	4.08	…	…	0.06	$^{13}CH_3CN$,CH_3OCOH v_t =1
tEME-EA	$8_{4,4}$–$7_{3,4}$	232 154.362	32.3	3.08	†			
tEME-EA	$8_{4,5}$–$7_{3,5}$	232 155.426	32.3	3.08	†			
tEME-AA	$8_{4,4}$–$7_{3,5}$	232 156.540	32.3	4.08	…	…	0.04	$^{13}CH_3CN$,CH_3OCOH v_t =1
tEME-EA	$8_{4,4}$–$7_{3,5}$	232 157.268	32.3	1.00	†			
tEME-EE	$14_{3,11}$–$13_{2,12}$	233 622.462	51.0	4.51	…	…	0.10	CH_3OCOH v_t = 0,1
tEME-EE’	$14_{3,11}$–$13_{2,12}$	233 622.556	51.0	4.51	†			
tEME-AE	$14_{3,11}$–$13_{2,12}$	233 622.806	51.0	4.51	†			
tEME-EA	$14_{3,11}$–$13_{2,12}$	233 624.824	51.0	4.52	…	…	0.06	CH_3OCOH v_t = 0,1
tEME-AA	$14_{3,11}$–$13_{2,12}$	233 625.121	51.0	4.52	†			
tEME-EA	$30_{0,30}$–$29_{1,29}$	234 130.523	177.0	24.66	…	…	0.27	CH_3CH_2CN v_{13}/v_{21}
tEME-AA	$30_{0,30}$–$29_{1,29}$	234 130.524	177.0	24.66	†			
tEME-EE	$30_{0,30}$–$29_{1,29}$	234 130.601	177.0	24.66	†			
tEME-EE’	$30_{0,30}$–$29_{1,29}$	234 130.601	177.0	24.66	†			
tEME-AE	$30_{0,30}$–$29_{1,29}$	234 130.602	177.0	24.66	†			
tEME-EE	$17_{2,15}$–$16_{1,16}$	235 247.484	64.0	2.37	235 247.6	0.09	0.05	
tEME-EE’	$17_{2,15}$–$16_{1,16}$	235 247.485	64.0	2.37	†			
tEME-AE	$17_{2,15}$–$16_{1,16}$	235 247.731	64.0	2.37	†			
tEME-EA	$17_{2,15}$–$16_{1,16}$	235 249.156	64.0	2.37	235 249.6	0.14	0.03	U-line
tEME-AA	$17_{2,15}$–$16_{1,16}$	235 249.403	64.0	2.37	†			
tEME-EE’	$25_{2,24}$–$24_{1,23}$	236 614.358	129.8	10.19	236 614.4	0.30	0.11	CH_3COOCH_3
tEME-EE	$25_{2,24}$–$24_{1,23}$	236 614.358	129.8	10.19	†			

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Species	Transition $J_{K_a,K_c} - J'_{K'_a,K'_c}$	Predicted frequency (MHz)	E_{upp} (K)	S_{ij}	Observed[1] frequency (MHz)	Observed[1] T_{MB} (K)	Model[2] T_{MB} (K)	Blends
tEME-AE	$25_{2,24}$–$24_{1,23}$	236 614.464	129.8	10.19	†			
tEME-EA	$25_{2,24}$–$24_{1,23}$	236 615.628	129.8	10.19	†		0.08	CH_3COOCH_3
tEME-AA	$25_{2,24}$–$24_{1,23}$	236 615.733	129.8	10.19	†			
tEME-AA	$32_{1,31}$–$31_{2,30}$	236 906.877	206.9	15.50	236 907.2	0.30	0.10	CH_3SH, HC_3N $v_6 = 1$
tEME-EA	$32_{1,31}$–$31_{2,30}$	236 906.908	206.9	15.50	†			
tEME-AE	$32_{1,31}$–$31_{2,30}$	236 907.656	206.9	15.50	†			
tEME-EE	$32_{1,31}$–$31_{2,30}$	236 907.687	206.9	15.50	†			
tEME-EE’	$32_{1,31}$–$31_{2,30}$	236 907.687	206.9	15.50	†			
tEME-EE’	$30_{1,30}$–$29_{0,29}$	237 763.517	177.1	24.69	237 763.6	0.48	0.28	CH_2CHCN
tEME-EE	$30_{1,30}$–$29_{0,29}$	237 763.517	177.1	24.69	†			
tEME-AE	$30_{1,30}$–$29_{0,29}$	237 763.527	177.1	24.69	†			
tEME-EA	$30_{1,30}$–$29_{0,29}$	237 763.653	177.1	24.69	†			
tEME-AA	$30_{1,30}$–$29_{0,29}$	237 763.664	177.1	24.69	†			
tEME-EE’	$15_{3,13}$–$14_{2,12}$	237 865.715	56.7	4.79	…	…	0.10	CH_2CHCN
tEME-EE	$15_{3,13}$–$14_{2,12}$	237 865.778	56.7	4.80	†			
tEME-AE	$15_{3,13}$–$14_{2,12}$	237 866.042	56.7	4.80	†			
tEME-EA	$15_{3,13}$–$14_{2,12}$	237 868.339	56.7	4.80	…	…	0.08	CH_2CHCN
tEME-AA	$15_{3,13}$–$14_{2,12}$	237 868.635	56.7	4.80	†			
tEME-EA	$9_{4,6}$–$8_{3,5}$	240 195.817	35.8	1.64	…	…	0.10	CH_2CHCN $v_{15} = 1$
tEME-EE	$9_{4,5}$–$8_{3,5}$	240 196.101	35.8	3.88	†			
tEME-EE’	$9_{4,6}$–$8_{3,6}$	240 196.396	35.8	3.88	†			
tEME-EE’	$9_{4,5}$–$8_{3,5}$	240 196.642	35.8	3.88	†			
tEME-AE	$9_{4,5}$–$8_{3,5}$	240 196.777	35.8	3.88	†			
tEME-EE	$9_{4,6}$–$8_{3,6}$	240 196.937	35.8	3.88	†			
tEME-AE	$9_{4,6}$–$8_{3,6}$	240 197.045	35.8	3.88	†			
tEME-AA	$9_{4,6}$–$8_{3,5}$	240 197.196	35.8	3.88	†			
tEME-EA	$9_{4,5}$–$8_{3,5}$	240 197.654	35.8	3.88	†			
tEME-EA	$9_{4,6}$–$8_{3,6}$	240 201.478	35.8	2.63	…	…	0.05	CH_2CHCN $v_{15} = 1$
tEME-AA	$9_{4,5}$–$8_{3,6}$	240 202.719	35.8	4.28	†			
tEME-EA	$9_{4,5}$–$8_{3,6}$	240 203.315	35.8	1.64	†			
tEME-EE	$15_{3,12}$–$14_{2,13}$	242 035.318	56.8	4.68	…	…	0.10	CH_2DCN
tEME-EE’	$15_{3,12}$–$14_{2,13}$	242 035.380	56.8	4.68	†			
tEME-AE	$15_{3,12}$–$14_{2,13}$	242 035.647	56.8	4.68	†			
tEME-EA	$15_{3,12}$–$14_{2,13}$	242 037.704	56.8	4.68			0.07	CH_2DCN
tEME-EA	$15_{3,12}$–$14_{2,13}$	242 038.002	56.8	4.68	†			
tEME-EE’	$26_{2,25}$–$25_{1,24}$	242 161.785	139.8	10.89	…	…	0.32	CH_3CH_2CN $v_{20} = 1$
tEME-EE	$26_{2,25}$–$25_{1,24}$	242 161.785	139.8	10.89	†			
tEME-AE	$26_{2,25}$–$25_{1,24}$	242 161.884	139.8	10.89	†			
tEME-EA	$26_{2,25}$–$25_{1,24}$	242 163.015	139.8	10.89	†			
tEME-AA	$26_{2,25}$–$25_{1,24}$	242 163.114	139.8	10.89	†			
tEME-EA	$31_{0,31}$–$30_{1,30}$	242 163.369	188.7	25.69	†			

Species	Transition $J_{K_a,K_c} - J'_{K'_a,K'_c}$	Predicted frequency (MHz)	E_{upp} (K)	S_{ij}	Observed[1] frequency (MHz)	Observed[1] T_{MB} (K)	Model[2] T_{MB} (K)	Blends
tEME-AA	$31_{0,31}$–$30_{1,30}$	242 163.371	188.7	25.69	†			
tEME-EE	$31_{0,31}$–$30_{1,30}$	242 163.434	188.7	25.69	†			
tEME-EE’	$31_{0,31}$–$30_{1,30}$	242 163.434	188.7	25.69	†			
tEME-AE	$31_{0,31}$–$30_{1,30}$	242 163.436	188.7	25.69	†			
tEME-EE’	$16_{3,14}$–$15_{2,13}$	245 103.550	62.9	4.99	…	…	0.10	$CH_3CH_2{}^{13}CN$
tEME-EE	$16_{3,14}$–$15_{2,13}$	245 103.592	62.9	4.99	†			
tEME-AE	$16_{3,14}$–$15_{2,13}$	245 103.864	62.9	4.99	†			
tEME-EA	$16_{3,14}$–$15_{2,13}$	245 106.133	62.9	4.99	245 106.4	0.32	0.07	CH_2OHCHO
tEME-AA	$16_{3,14}$–$15_{2,13}$	245 106.426	62.9	5.00	†			
tEME-EE’	$31_{1,31}$–$30_{0,30}$	245 274.088	188.8	25.71	245 274.3	0.40	0.29	$^{34}SO_2$
tEME-EE	$31_{1,31}$–$30_{0,30}$	245 274.088	188.8	25.71	†			
tEME-AE	$31_{1,31}$–$30_{0,30}$	245 274.098	188.8	25.71	†			
tEME-EA	$31_{1,31}$–$30_{0,30}$	245 274.211	188.8	25.71	†			
tEME-AA	$31_{1,31}$–$30_{0,30}$	245 274.221	188.8	25.71	†			
tEME-AA	$33_{1,32}$–$32_{2,31}$	246 605.346	219.6	16.51	246 606.0	0.36	0.11	CH_3OCH_3
tEME-EA	$33_{1,32}$–$32_{2,31}$	246 605.372	219.6	16.51	†			
tEME-AE	$33_{1,32}$–$32_{2,31}$	246 606.066	219.6	16.51	†			
tEME-EE	$33_{1,32}$–$32_{2,31}$	246 606.092	219.6	16.51	†			
tEME-EE’	$33_{1,32}$–$32_{2,31}$	246 606.092	219.6	16.51	†			
tEME-EE	$18_{2,16}$–$17_{1,17}$	247 478.246	71.1	2.26	247 478.0	0.16	0.05	CH_3OCOH $v_t = 1$
tEME-EE’	$18_{2,16}$–$17_{1,17}$	247 478.247	71.1	2.26	†			
tEME-AE	$18_{2,16}$–$17_{1,17}$	247 478.501	71.1	2.26	†			
tEME-EA	$18_{2,16}$–$17_{1,17}$	247 479.920	71.1	2.26	247 480.0	0.16	0.03	CH_3OCOH $v_t = 1$
tEME-AA	$18_{2,16}$–$17_{1,17}$	247 480.175	71.1	2.26	†			
tEME-EE’	$27_{2,26}$–$26_{1,25}$	247 721.097	150.2	11.63	247 721.2	0.23	0.11	
tEME-EE	$27_{2,26}$–$26_{1,25}$	247 721.097	150.2	11.63	†			
tEME-AE	$27_{2,26}$–$26_{1,25}$	247 721.190	150.2	11.63	†			
tEME-EA	$27_{2,26}$–$26_{1,25}$	247 722.285	150.2	11.63	†			
tEME-AA	$27_{2,26}$–$26_{1,25}$	247 722.378	150.2	11.63	†			
tEME-EA	$10_{4,7}$–$9_{3,6}$	248 234.223	39.7	2.12	248 235.7	0.31	0.15	U-line
tEME-EE	$10_{4,6}$–$9_{3,6}$	248 235.232	39.7	3.50	†			
tEME-AA	$10_{4,7}$–$9_{3,6}$	248 235.506	39.7	4.48	†			
tEME-EA	$10_{4,6}$–$9_{3,6}$	248 236.059	39.7	2.36	†			
tEME-AE	$10_{4,6}$–$9_{3,6}$	248 236.076	39.7	3.66	†			
tEME-EE’	$10_{4,6}$–$9_{3,6}$	248 236.093	39.7	3.79	†			
tEME-EE’	$10_{4,7}$–$9_{3,7}$	248 239.115	39.7	3.79	248 239.8	0.07	0.09	U-line
tEME-AE	$10_{4,7}$–$9_{3,7}$	248 239.913	39.7	3.66	†			
tEME-EE	$10_{4,7}$–$9_{3,7}$	248 239.977	39.7	3.50	†			
tEME-EA	$10_{4,7}$–$9_{3,7}$	248 245.234	39.7	2.36	…	…	0.06	CH_3COCH_3
tEME-AA	$10_{4,6}$–$9_{3,7}$	248 246.569	39.7	4.48	†			
tEME-EA	$10_{4,6}$–$9_{3,7}$	248 247.070	39.7	2.12	†			

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Species	Transition $J_{K_a,K_c} - J'_{K'_a,K'_c}$	Predicted frequency (MHz)	E_{upp} (K)	S_{ij}	Observed[1] frequency (MHz)	Observed[1] T_{MB} (K)	Model[2] T_{MB} (K)	Blends
tEME-EE	$10_{4,6}–9_{3,7}$	248 248.602	39.7	0.98	†			
tEME-AE	$10_{4,6}–9_{3,7}$	248 250.368	39.7	0.82	†			
tEME-EE’	$10_{4,6}–9_{3,7}$	248 251.399	39.7	0.69	†			
tEME-EA	$32_{0,32}–31_{1,31}$	250 160.753	200.8	26.72	…	…	0.29	$^{34}SO_2$
tEME-AA	$32_{0,32}–31_{1,31}$	250 160.756	200.8	26.72	†			
tEME-EE	$32_{0,32}–31_{1,31}$	250 160.807	200.8	26.72	†			
tEME-EE’	$32_{0,32}–31_{1,31}$	250 160.807	200.8	26.72	†			
tEME-AE	$32_{0,32}–31_{1,31}$	250 160.810	200.8	26.72	†			
tEME-EE	$16_{3,13}–15_{2,14}$	250 534.903	62.9	4.83	250 535.0	0.16	0.11	
tEME-EE’	$16_{3,13}–15_{2,14}$	250 534.946	62.9	4.83	†			
tEME-AE	$16_{3,13}–15_{2,14}$	250 535.223	62.9	4.83	†			
tEME-EA	$16_{3,13}–15_{2,14}$	250 537.299	62.9	4.83	250 537.5	0.11	0.08	
tEME-AA	$16_{3,13}–15_{2,14}$	250 537.598	62.9	4.83	†			
tEME-EE’	$17_{3,15}–16_{2,14}$	252 188.288	69.5	5.19	252 188.5	0.59	0.11	CH_3CH_2CN v_{13}/v_{21}
tEME-EE	$17_{3,15}–16_{2,14}$	252 188.318	69.5	5.19	†			
tEME-AE	$17_{3,15}–16_{2,14}$	252 188.592	69.5	5.19	†			
tEME-EA	$17_{3,15}–16_{2,14}$	252 190.846	69.5	5.19	…	…	0.08	CH_3CH_2CN v_{13}/v_{21}
tEME-AA	$17_{3,15}–16_{2,14}$	252 191.135	69.5	5.19	†			
tEME-EE’	$32_{1,32}–31_{0,31}$	252 818.715	200.8	26.74	…	…	0.29	CH_3OH
tEME-EE	$32_{1,32}–31_{0,31}$	252 818.715	200.8	26.74	†			
tEME-AE	$32_{1,32}–31_{0,31}$	252 818.724	200.8	26.74	†			
tEME-EA	$32_{1,32}–31_{0,31}$	252 818.826	200.8	26.74	†			
tEME-AA	$32_{1,32}–31_{0,31}$	252 818.835	200.8	26.74	†			
tEME-EE’	$28_{2,27}–27_{1,26}$	253 307.713	161.0	12.42	…	…	0.12	$^{13}CH_3OH$
tEME-EE	$28_{2,27}–27_{1,26}$	253 307.713	161.0	12.42	†			
tEME-AE	$28_{2,27}–27_{1,26}$	253 307.800	161.0	12.42	†			
tEME-EA	$28_{2,27}–27_{1,26}$	253 308.856	161.0	12.42	†			
tEME-AA	$28_{2,27}–27_{1,26}$	253 308.943	161.0	12.42	†			
tEME-EE	$5_{5,0}–4_{4,0}$	255 923.090	34.6	4.50	255 923.1	0.42	0.29	CH_3CH_2CN
tEME-EE’	$5_{5,1}–4_{4,1}$	255 923.151	34.6	4.50	†			
tEME-EE’	$5_{5,0}–4_{4,0}$	255 923.293	34.6	4.50	†			
tEME-EE	$5_{5,1}–4_{4,1}$	255 923.354	34.6	4.50	†			
tEME-AE	$5_{5,0}–4_{4,0}$	255 923.648	34.6	4.50	†			
tEME-AE	$5_{5,1}–4_{4,1}$	255 923.709	34.6	4.50	†			
tEME-EA	$5_{5,1}–4_{4,1}$	255 926.362	34.6	4.50	255 926.5	0.37	0.20	SO_2
tEME-EA	$5_{5,0}–4_{4,0}$	255 926.565	34.6	4.50	†			
tEME-AA	$5_{5,1}–4_{4,0}$	255 926.920	34.6	4.50	†			
tEME-AA	$5_{5,0}–4_{4,1}$	255 926.920	34.6	4.50	†			
tEME-AA	$34_{1,33}–33_{2,32}$	256 180.110	232.7	17.54	256 180.5	0.28	0.11	CH_3OCOH $v_t = 1$
tEME-EA	$34_{1,33}–33_{2,32}$	256 180.131	232.7	17.54	†			
tEME-AE	$34_{1,33}–33_{2,32}$	256 180.771	232.7	17.54	†			

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Species	Transition $J_{K_a,K_c} - J'_{K'_a,K'_c}$	Predicted frequency (MHz)	E_{upp} (K)	S_{ij}	Observed[1] frequency (MHz)	Observed[1] T_{MB} (K)	Model[2] T_{MB} (K)	Blends
tEME-EE	$34_{1,33}$–$33_{2,32}$	256 180.792	232.7	17.54	†			
tEME-EE’	$34_{1,33}$–$33_{2,32}$	256 180.792	232.7	17.54	†			
tEME-EA	$11_{4,8}$–$10_{3,7}$	256 265.991	43.9	2.59	…	…	0.10	SO_2
tEME-AA	$11_{4,8}$–$10_{3,7}$	256 267.169	43.9	4.68	†			
tEME-EE	$11_{4,7}$–$10_{3,7}$	256 267.504	43.9	3.09	†			
tEME-EA	$11_{4,7}$–$10_{3,7}$	256 267.843	43.9	2.09	†			
tEME-AE	$11_{4,8}$–$10_{3,8}$	256 280.321	43.9	3.24	…	…	0.07	CH_3OCOH $v_t = 1$
tEME-EE	$11_{4,8}$–$10_{3,8}$	256 280.554	43.9	3.09	†			
tEME-AE	$11_{4,7}$–$10_{3,8}$	256 290.759	43.9	1.44	…	…	0.07	CH_3CCH
tEME-EE’	$11_{4,7}$–$10_{3,8}$	256 291.611	43.9	1.30	†			
tEME-EA	$33_{0,33}$–$32_{1,32}$	258 126.741	213.2	27.74	…	…	0.29	CH_3CN $v_8 = 1$,CH_3OCOH
tEME-AA	$33_{0,33}$–$32_{1,32}$	258 126.744	213.2	27.74	†			
tEME-EE	$33_{0,33}$–$32_{1,32}$	258 126.784	213.2	27.74	†			
tEME-EE’	$33_{0,33}$–$32_{1,32}$	258 126.784	213.2	27.74	†			
tEME-AE	$33_{0,33}$–$32_{1,32}$	258 126.787	213.2	27.74	†			
tEME-EE’	$29_{2,28}$–$28_{1,27}$	258 936.835	172.1	13.24	…	…	0.12	SO_2
tEME-EE	$29_{2,28}$–$28_{1,27}$	258 936.835	172.1	13.24	†			
tEME-AE	$29_{2,28}$–$28_{1,27}$	258 936.915	172.1	13.24	†			
tEME-EA	$29_{2,28}$–$28_{1,27}$	258 937.931	172.1	13.24	†			
tEME-AA	$29_{2,28}$–$28_{1,27}$	258 938.012	172.1	13.24	†			
tEME-EE’	$18_{3,16}$–$17_{2,15}$	259 109.696	76.5	5.39	…	…	0.11	CH_3OCOH
tEME-EE	$18_{3,16}$–$17_{2,15}$	259 109.717	76.5	5.39	†			
tEME-AE	$18_{3,16}$–$17_{2,15}$	259 109.992	76.5	5.39	†			
tEME-EA	$18_{3,16}$–$17_{2,15}$	259 112.236	76.5	5.39	…	…	0.08	CH_3OCOH
tEME-AA	$18_{3,16}$–$17_{2,15}$	259 112.522	76.5	5.39	†			
tEME-EE	$17_{3,14}$–$16_{2,15}$	259 135.164	69.5	4.97	…	…	0.11	CH_3OCOH
tEME-EE’	$17_{3,14}$–$16_{2,15}$	259 135.193	69.5	4.97	†			
tEME-AE	$17_{3,14}$–$16_{2,15}$	259 135.477	69.5	4.97	†			
tEME-EA	$17_{3,14}$–$16_{2,15}$	259 137.561	69.5	4.97	…	…	0.08	CH_3OCOH
tEME-AA	$17_{3,14}$–$16_{2,15}$	259 137.860	69.5	4.97	†			
tEME-EE	$19_{2,17}$–$18_{1,18}$	260 106.865	78.5	2.13	…	…	0.05	CH_3CH_2OH
tEME-EE’	$19_{2,17}$–$18_{1,18}$	260 106.865	78.5	2.13	†			
tEME-AE	$19_{2,17}$–$18_{1,18}$	260 107.129	78.5	2.13	†			
tEME-EA	$19_{2,17}$–$18_{1,18}$	260 108.541	78.5	2.13	…	…	0.05	CH_3CH_2OH
tEME-AA	$19_{2,17}$–$18_{1,18}$	260 108.805	78.5	2.13	†			
tEME-EE’	$33_{1,33}$–$32_{0,32}$	260 393.451	213.3	27.76	…	…	0.29	CH_3OCOH
tEME-EE	$33_{1,33}$–$32_{0,32}$	260 393.451	213.3	27.76	†			
tEME-AE	$33_{1,33}$–$32_{0,32}$	260 393.460	213.3	27.76	†			
tEME-EA	$33_{1,33}$–$32_{0,32}$	260 393.552	213.3	27.76	†			
tEME-AA	$33_{1,33}$–$32_{0,32}$	260 393.560	213.3	27.76	†			
tEME-EE’	$40_{6,35}$–$40_{5,36}$	260 504.644	358.5	20.96	…	…		SiO

Species	Transition $J_{K_a,K_c} - J'_{K'_a,K'_c}$	Predicted frequency (MHz)	E_{upp} (K)	S_{ij}	Observed[1] frequency (MHz)	Observed[1] T_{MB} (K)	Model[2] T_{MB} (K)	Blends
tEME-EE	$40_{6,35}$–$40_{5,36}$	260 505.033	358.5	21.22	†			
tEME-AE	$40_{6,35}$–$40_{5,36}$	260 505.210	358.5	21.10	†			
tEME-EA	$40_{6,35}$–$40_{5,36}$	260 507.959	358.5	21.43	†			
tEME-AA	$40_{6,35}$–$40_{5,36}$	260 508.333	358.5	21.45	†			
tEME-EE	$38_{6,32}$–$38_{5,33}$	260 681.821	327.9	19.53	…	…	0.03	CH_3CH_2CN
tEME-AE	$38_{6,32}$–$38_{5,33}$	260 682.506	327.9	19.20	†			
tEME-EE’	$38_{6,32}$–$38_{5,33}$	260 682.515	327.9	18.84	†			
tEME-EA	$38_{6,32}$–$38_{5,33}$	260 683.965	327.9	20.17	†			
tEME-AA	$38_{6,32}$–$38_{5,33}$	260 684.291	327.9	20.22	†			
tEME-EE	$37_{6,31}$–$37_{5,32}$	261 001.915	313.2	18.45	…	…	0.03	$OC^{34}S$, CH_3OCOH
tEME-AE	$37_{6,31}$–$37_{5,32}$	261 002.704	313.2	17.96	†			
tEME-EE’	$37_{6,31}$–$37_{5,32}$	261 002.807	313.2	17.46	†			
tEME-EE’	$38_{6,33}$–$38_{5,34}$	261 029.561	327.9	18.84	261 030.4	0.27	0.03	CH_3OCOH $v_t = 1$
tEME-EE	$38_{6,33}$–$38_{5,34}$	261 030.255	327.9	19.53	†			
tEME-AE	$38_{6,33}$–$38_{5,34}$	261 030.302	327.9	19.20	†			
tEME-EA	$38_{6,33}$–$38_{5,34}$	261 033.470	327.9	20.16	…	…	0.03	CH_3OCOH
tEME-AA	$38_{6,33}$–$38_{5,34}$	261 033.876	327.9	20.22	†			
tEME-EE’	$37_{6,32}$–$37_{5,33}$	261 270.008	313.2	17.46	…	…	0.03	CH_3CH_2CN v_{13}/v_{21}
tEME-AE	$37_{6,32}$–$37_{5,33}$	261 270.856	313.2	17.95	†			
tEME-EE	$37_{6,32}$–$37_{5,33}$	261 270.899	313.2	18.45	†			
tEME-AE	$36_{6,30}$–$36_{5,31}$	261 291.812	298.9	16.50	…	…	0.04	CH_3CH_2OH
tEME-EE’	$36_{6,30}$–$36_{5,31}$	261 292.008	298.9	15.92	†			
tEME-EA	$36_{6,30}$–$36_{5,31}$	261 292.672	298.9	18.82	†			
tEME-AA	$36_{6,30}$–$36_{5,31}$	261 292.970	298.9	19.00	†			
tEME-AE	$36_{6,31}$–$36_{5,32}$	261 496.448	298.9	16.50	…	…	0.03	CH_2CN
tEME-EE	$36_{6,31}$–$36_{5,32}$	261 496.589	298.9	17.15	†			
tEME-EA	$36_{6,31}$–$36_{5,32}$	261 500.259	298.9	18.82	…	…	0.03	CH_3OCOH, CH_2CN
tEME-AA	$36_{6,31}$–$36_{5,32}$	261 500.719	298.9	19.00	†			
tEME-EE’	$35_{6,29}$–$35_{5,30}$	261 553.036	285.0	14.38	261 553.2	0.15	0.06	$CH_3O^{13}COH$ $v_t = 1$
tEME-EA	$35_{6,29}$–$35_{5,30}$	261 553.277	285.0	18.06	†			
tEME-AA	$35_{6,29}$–$35_{5,30}$	261 553.546	285.0	18.40	†			
tEME-AE	$35_{6,30}$–$35_{5,31}$	261 707.095	285.0	14.94	…	…	0.03	CH_3OH
tEME-EE	$35_{6,30}$–$35_{5,31}$	261 707.325	285.0	15.65	†			
tEME-EA	$35_{6,30}$–$35_{5,31}$	261 711.277	285.0	18.06	…	…	0.03	CH_3OCOH
tEME-AA	$35_{6,30}$–$35_{5,31}$	261 711.778	285.0	18.40	†			
tEME-EE	$34_{6,28}$–$34_{5,29}$	261 787.091	271.4	14.12	…	…	0.07	CH_3OCOH, CH_3OH, SO
tEME-AE	$34_{6,28}$–$34_{5,29}$	261 788.168	271.4	13.47	†			
tEME-EA	$34_{6,28}$–$34_{5,29}$	261 788.351	271.4	17.16	†			
tEME-EE’	$34_{6,28}$–$34_{5,29}$	261 788.486	271.4	13.02	†			
tEME-AA	$34_{6,28}$–$34_{5,29}$	261 788.577	271.4	17.80	†			
tEME-EE’	$34_{6,29}$–$34_{5,30}$	261 901.878	271.4	13.02	…	…	0.03	CH_3OCH_3,CH_3COCH_3

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Species	Transition $J_{K_a,K_c} - J'_{K'_a,K'_c}$	Predicted frequency (MHz)	E_{upp} (K)	S_{ij}	Observed[1] frequency (MHz)	Observed[1] T_{MB} (K)	Model[2] T_{MB} (K)	Blends
tEME-AE	$34_{6,29}$–$34_{5,30}$	261 902.977	271.4	13.47	†			
tEME-EE	$34_{6,29}$–$34_{5,30}$	261 903.273	271.4	14.12	†			
tEME-EA	$34_{6,29}$–$34_{5,30}$	261 907.508	271.4	17.16	…	…	0.03	CH_3OCH_3,CH_3COCH_3
tEME-AA	$34_{6,29}$–$34_{5,30}$	261 908.064	271.4	17.80	†			
tEME-EA	$33_{6,27}$–$33_{5,29}$	262 000.261	258.3	16.05	…	…	0.08	CCH
tEME-AE	$33_{6,27}$–$33_{5,29}$	262 000.337	258.3	12.24	†			
tEME-AA	$33_{6,27}$–$33_{5,29}$	262 000.424	258.3	17.21	†			
tEME-EE'	$33_{6,27}$–$33_{5,29}$	262 000.673	258.3	11.95	†			
tEME-AE	$33_{6,27}$–$33_{5,29}$	262 084.400	258.3	12.24	…	…	0.03	CH_3OCOH
tEME-EE	$33_{6,27}$–$33_{5,29}$	262 084.731	258.3	12.72	†			
tEME-EA	$33_{6,27}$–$33_{5,29}$	262 089.211	258.3	16.05	…	…	0.03	CH_3OCOH
tEME-AA	$33_{6,27}$–$33_{5,29}$	262 089.841	258.3	17.21	†			
tEME-EA	$32_{6,27}$–$32_{5,28}$	262 191.119	245.5	14.67	…	…	0.08	CH_3CH_2CN
tEME-AA	$32_{6,26}$–$32_{5,28}$	262 191.200	245.5	16.62	†			
tEME-AE	$32_{6,26}$–$32_{5,28}$	262 191.354	245.5	11.34	†			
tEME-EE'	$32_{6,26}$–$32_{5,28}$	262 191.682	245.5	11.22	†			
tEME-AE	$32_{6,27}$–$32_{5,28}$	262 251.766	245.5	11.34	…	…	0.04	SO_2
tEME-EE	$32_{6,27}$–$32_{5,28}$	262 252.104	245.5	11.61	†			
tEME-EA	$32_{6,27}$–$32_{5,28}$	262 256.756	245.5	14.67	…	…	0.04	SO_2
tEME-AA	$32_{6,27}$–$32_{5,28}$	262 257.479	245.5	16.62	†			
tEME-AE	$32_{6,26}$–$32_{5,28}$	262 260.269	245.5	5.28	†			
tEME-EE'	$32_{6,26}$–$32_{5,28}$	262 260.849	245.5	5.41	†			
tEME-AA	$31_{6,25}$–$31_{5,26}$	262 362.797	233.1	16.04	…	…	0.08	$CH_3{}^{13}CH_2CN$
tEME-EA	$31_{6,25}$–$31_{5,26}$	262 362.814	233.1	13.11	†			
tEME-AE	$31_{6,25}$–$31_{5,26}$	262 363.092	233.1	10.77	†			
tEME-EE'	$31_{6,25}$–$31_{5,26}$	262 363.388	233.1	10.80	†			
tEME-EE'	$31_{6,26}$–$31_{5,27}$	262 404.436	233.1	10.80	…	…	0.04	$^{13}CH_3OCOH$ $v_t = 1$
tEME-AE	$31_{6,26}$–$31_{5,27}$	262 405.547	233.1	10.77	†			
tEME-EE	$31_{6,25}$–$31_{5,27}$	262 405.867	233.1	10.84	†			
tEME-EA	$31_{6,26}$–$31_{5,27}$	262 410.601	233.1	13.11	…	…	0.04	$^{13}CH_3OCOH$ $v_t = 1$
tEME-AA	$31_{6,26}$–$31_{5,27}$	262 411.432	233.1	16.04	†			
tEME-EA	$30_{6,25}$–$30_{5,25}$	262 515.014	221.2	3.88	…	…	0.09	U-line
tEME-EE	$30_{6,24}$–$30_{5,25}$	262 516.140	221.2	10.39	†			
tEME-AA	$30_{6,24}$–$30_{5,25}$	262 516.918	221.2	15.45	†			
tEME-EA	$30_{6,24}$–$30_{5,25}$	262 517.034	221.2	11.57	†			
tEME-AE	$30_{6,24}$–$30_{5,25}$	262 517.242	221.2	10.51	†			
tEME-EE'	$30_{6,24}$–$30_{5,25}$	262 517.483	221.2	10.68	†			
tEME-EE'	$30_{6,25}$–$30_{5,26}$	262 545.215	221.2	10.68	…	…	0.04	H_2CCO
tEME-AE	$30_{6,25}$–$30_{5,26}$	262 546.281	221.2	10.51	†			
tEME-EE	$30_{6,25}$–$30_{5,26}$	262 546.558	221.2	10.39	†			
tEME-EA	$30_{6,25}$–$30_{5,26}$	262 551.283	221.2	11.57	…	…	0.04	H_2CCO

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Species	Transition $J_{K_a,K_c} - J'_{K'_a,K'_c}$	Predicted frequency (MHz)	E_{upp} (K)	S_{ij}	Observed[1] frequency (MHz)	Observed[1] T_{MB} (K)	Model[2] T_{MB} (K)	Blends
tEME-AA	$30_{6,25}$–$30_{5,26}$	262 552.224	221.2	15.45	†			
tEME-EE	$30_{6,24}$–$30_{5,26}$	262 553.207	221.2	5.06	†			
tEME-EA	$30_{6,24}$–$30_{5,26}$	262 553.303	221.2	3.88	†			
tEME-EE	$29_{6,23}$–$29_{5,24}$	262 654.283	209.6	10.25	…	…	0.10	CH_3COCH_3
tEME-AA	$29_{6,23}$–$29_{5,24}$	262 655.095	209.6	14.87	†			
tEME-EA	$29_{6,23}$–$29_{5,24}$	262 655.300	209.6	10.29	†			
tEME-AE	$29_{6,23}$–$29_{5,24}$	262 655.326	209.6	10.53	†			
tEME-EE’	$29_{6,23}$–$29_{5,24}$	262 655.485	209.6	10.83	†			
tEME-EE’	$29_{6,24}$–$29_{5,25}$	262 673.561	209.6	10.83	…	…	0.05	$HC^{13}CCN$
tEME-AE	$29_{6,24}$–$29_{5,25}$	262 674.556	209.6	10.53	†			
tEME-EE	$29_{6,24}$–$29_{5,25}$	262 674.763	209.6	10.25	†			
tEME-EA	$29_{6,24}$–$29_{5,25}$	262 679.394	209.6	10.29	…	…	0.04	$HC^{13}CCN$
tEME-AA	$29_{6,24}$–$29_{5,25}$	262 680.434	209.6	14.87	†			
tEME-EA	$29_{6,23}$–$29_{5,25}$	262 681.315	209.6	4.58	†			
tEME-EE	$29_{6,23}$–$29_{5,25}$	262 681.410	209.6	4.63	†			
tEME-EA	$28_{6,23}$–$28_{5,23}$	262 777.103	198.3	4.94	…	…	0.10	CH_3OCH_3
tEME-EE	$28_{6,22}$–$28_{5,23}$	262 777.763	198.3	10.37	†			
tEME-AA	$28_{6,22}$–$28_{5,23}$	262 778.714	198.3	14.30	†			
tEME-AE	$28_{6,22}$–$28_{5,23}$	262 778.719	198.3	10.78	†			
tEME-EE’	$28_{6,22}$–$28_{5,23}$	262 778.771	198.3	11.17	†			
tEME-EA	$28_{6,22}$–$28_{5,23}$	262 778.988	198.3	9.35	†			
tEME-EE’	$28_{6,23}$–$28_{5,24}$	262 790.103	198.3	11.17	262 791.0	0.25	0.05	U-line
tEME-AE	$28_{6,23}$–$28_{5,24}$	262 791.000	198.3	10.78	†			
tEME-EE	$28_{6,23}$–$28_{5,24}$	262 791.111	198.3	10.37	†			
tEME-EA	$28_{6,23}$–$28_{5,24}$	262 795.561	198.3	9.35	…	…	0.04	CH_2OHCHO
tEME-AA	$28_{6,23}$–$28_{5,24}$	262 796.681	198.3	14.30	†			
tEME-EA	$28_{6,22}$–$28_{5,24}$	262 797.446	198.3	4.94	†			
tEME-EE	$28_{6,22}$–$28_{5,24}$	262 797.772	198.3	3.92	†			
tEME-EA	$27_{6,22}$–$27_{5,22}$	262 887.474	187.5	4.97	…	…	0.10	CH_3COOH, CH_3OCH_3
tEME-EE	$27_{6,21}$–$27_{5,22}$	262 887.831	187.5	10.70	†			
tEME-EE’	$27_{6,21}$–$27_{5,22}$	262 888.603	187.5	11.58	†			
tEME-AE	$27_{6,21}$–$27_{5,22}$	262 888.676	187.5	11.18	†			
tEME-AA	$27_{6,21}$–$27_{5,22}$	262 889.035	187.5	13.72	†			
tEME-EA	$27_{6,21}$–$27_{5,22}$	262 889.353	187.5	8.75	†			
tEME-EE’	$27_{6,22}$–$27_{5,23}$	262 895.483	187.5	11.58	…	…	0.07	CH_3OCH_3
tEME-EE	$27_{6,22}$–$27_{5,23}$	262 896.256	187.5	10.70	†			
tEME-AE	$27_{6,22}$–$27_{5,23}$	262 896.265	187.5	11.18	†			
tEME-EA	$27_{6,22}$–$27_{5,23}$	262 900.436	187.5	8.75	…	…	0.05	CH_3COOH
tEME-AA	$27_{6,22}$–$27_{5,23}$	262 901.609	187.5	13.72	†			
tEME-EA	$27_{6,21}$–$27_{5,23}$	262 902.316	187.5	4.97	†			
tEME-EE	$27_{6,21}$–$27_{5,23}$	262 902.939	187.5	3.02	†			

Species	Transition $J_{K_a,K_c} - J'_{K'_a,K'_c}$	Predicted frequency (MHz)	E_{upp} (K)	S_{ij}	Observed[1] frequency (MHz)	Observed[1] T_{MB} (K)	Model[2] T_{MB} (K)	Blends
tEME-EE	$26_{6,20}$–$26_{5,21}$	262 985.638	177.1	11.11	…	…	0.10	$CH_3{}^{18}OH$
tEME-EA	$26_{6,21}$–$26_{5,21}$	262 985.653	177.1	4.68	†			
tEME-EE’	$26_{6,20}$–$26_{5,21}$	262 986.169	177.1	11.87	†			
tEME-AE	$26_{6,20}$–$26_{5,21}$	262 986.363	177.1	11.54	†			
tEME-AA	$26_{6,20}$–$26_{5,21}$	262 987.205	177.1	13.15	†			
tEME-EA	$26_{6,20}$–$26_{5,21}$	262 987.541	177.1	8.47	†			
tEME-EE’	$26_{6,21}$–$26_{5,22}$	262 990.328	177.1	11.87	…	…	0.09	$CH_3{}^{18}OH$
tEME-EE	$26_{6,21}$–$26_{5,22}$	262 990.859	177.1	11.11	†			
tEME-AE	$26_{6,21}$–$26_{5,22}$	262 990.997	177.1	11.54	†			
tEME-EA	$26_{6,21}$–$26_{5,22}$	262 994.684	177.1	8.47	…	…	0.05	SO_2 $v_2 = 1$
tEME-AA	$26_{6,21}$–$26_{5,22}$	262 995.883	177.1	13.15	†			
tEME-EA	$26_{6,20}$–$26_{5,22}$	262 996.572	177.1	4.68	†			
tEME-EE	$26_{6,20}$–$26_{5,22}$	262 997.567	177.1	2.04	†			
tEME-EE	$25_{6,19}$–$25_{5,20}$	263 072.263	167.0	11.39	…	…	0.11	U-line
tEME-EE’	$25_{6,19}$–$25_{5,20}$	263 072.594	167.0	11.92	†			
tEME-EA	$25_{6,20}$–$25_{5,20}$	263 072.699	167.0	4.12	†			
tEME-AE	$25_{6,19}$–$25_{5,20}$	263 072.885	167.0	11.70	†			
tEME-AA	$25_{6,19}$–$25_{5,20}$	263 074.277	167.0	12.58	…	…	0.11	U-line
tEME-EA	$25_{6,19}$–$25_{5,20}$	263 074.602	167.0	8.46	†			
tEME-EE’	$25_{6,20}$–$25_{5,21}$	263 075.234	167.0	11.92	†			
tEME-EE	$25_{6,20}$–$25_{5,21}$	263 075.564	167.0	11.39	†			
tEME-AE	$25_{6,20}$–$25_{5,21}$	263 075.815	167.0	11.70	†			
tEME-EA	$25_{6,20}$–$25_{5,21}$	263 078.980	167.0	8.46	…	…	0.05	U-line
tEME-AA	$25_{6,20}$–$25_{5,21}$	263 080.176	167.0	12.58	†			
tEME-EE	$24_{6,19}$–$24_{5,19}$	263 141.974	157.4	0.60	263 149.1	0.44	0.11	$CH_3O^{13}COH$,CH_3OCOD
tEME-EE	$24_{6,18}$–$24_{5,19}$	263 148.731	157.4	11.41	†			
tEME-EE’	$24_{6,18}$–$24_{5,19}$	263 148.928	157.4	11.70	†			
tEME-AE	$24_{6,18}$–$24_{5,19}$	263 149.281	157.4	11.59	†			
tEME-EA	$24_{6,19}$–$24_{5,19}$	263 149.579	157.4	3.30	†			
tEME-EE’	$24_{6,19}$–$24_{5,20}$	263 150.791	157.4	11.70	263 151.0	0.58	0.20	$CH_3O^{13}COH$,CH_3OCOD
tEME-EE	$24_{6,19}$–$24_{5,20}$	263 150.988	157.4	11.41	†			
tEME-AA	$24_{6,18}$–$24_{5,19}$	263 151.216	157.4	12.01	†			
tEME-AE	$24_{6,19}$–$24_{5,20}$	263 151.318	157.4	11.59	†			
tEME-EA	$24_{6,18}$–$24_{5,19}$	263 151.498	157.4	8.71	†			
tEME-EA	$24_{6,19}$–$24_{5,20}$	263 153.999	157.4	8.71	†			
tEME-AA	$24_{6,19}$–$24_{5,20}$	263 155.161	157.4	12.01	263 155.2	0.25	0.05	CH_3OCOD
tEME-EA	$24_{6,18}$–$24_{5,20}$	263 155.918	157.4	3.30	†			
tEME-EE	$23_{6,17}$–$23_{5,18}$	263 215.996	148.1	11.17	263 216.3	0.58	0.14	SO_2
tEME-EE’	$23_{6,17}$–$23_{5,18}$	263 216.118	148.1	11.31	†			
tEME-AE	$23_{6,17}$–$23_{5,18}$	263 216.506	148.1	11.26	†			
tEME-EA	$23_{6,18}$–$23_{5,18}$	263 217.183	148.1	2.31	263 217.8	0.59	0.14	SO_2

Species	Transition $J_{K_a,K_c} - J'_{K'_a,K'_c}$	Predicted frequency (MHz)	E_{upp} (K)	S_{ij}	Observed[1] frequency (MHz)	Observed[1] T_{MB} (K)	Model[2] T_{MB} (K)	Blends
tEME-EE'	$23_{6,18}$–$23_{5,19}$	263 217.615	148.1	11.31	†			
tEME-EE	$23_{6,18}$–$23_{5,19}$	263 217.736	148.1	11.17	†			
tEME-AE	$23_{6,18}$–$23_{5,19}$	263 218.114	148.1	11.26	†			
tEME-AA	$23_{6,17}$–$23_{5,18}$	263 218.914	148.1	11.44	†			
tEME-EA	$23_{6,17}$–$23_{5,18}$	263 219.118	148.1	9.14	†			
tEME-EA	$23_{6,18}$–$23_{5,19}$	263 220.415	148.1	9.14	…	…	0.05	SO_2
tEME-AA	$23_{6,18}$–$23_{5,19}$	263 221.507	148.1	11.44	†			
tEME-EA	$23_{6,17}$–$23_{5,19}$	263 222.351	148.1	2.31	†			
tEME-EE	$22_{6,16}$–$22_{5,17}$	263 274.922	139.2	10.76	…	…	0.14	CH_3OCH_3
tEME-EE'	$22_{6,16}$–$22_{5,17}$	263 275.007	139.2	10.82	†			
tEME-AE	$22_{6,16}$–$22_{5,17}$	263 275.415	139.2	10.80	†			
tEME-EA	$22_{6,17}$–$22_{5,17}$	263 276.341	139.2	1.34	†			
tEME-EE'	$22_{6,17}$–$22_{5,18}$	263 276.343	139.2	10.82	†			
tEME-EE	$22_{6,17}$–$22_{5,18}$	263 276.429	139.2	10.76	†			
tEME-AE	$22_{6,17}$–$22_{5,18}$	263 276.831	139.2	10.80	†			
tEME-AA	$22_{6,16}$–$22_{5,17}$	263 278.199	139.2	10.88	…	…	0.11	CH_3OCH_3
tEME-EA	$22_{6,16}$–$22_{5,17}$	263 278.292	139.2	9.53	†			
tEME-EA	$22_{6,17}$–$22_{5,18}$	263 278.882	139.2	9.53	†			
tEME-AA	$22_{6,17}$–$22_{5,18}$	263 279.871	139.2	10.88	†			
tEME-EE	$21_{6,15}$–$21_{5,16}$	263 326.288	130.7	10.27	263 326.7	0.42	0.14	HC_3N $v_7 = 1$,CH_3COCH_3
tEME-EE'	$21_{6,15}$–$21_{5,16}$	263 326.357	130.7	10.29	†			
tEME-AE	$21_{6,15}$–$21_{5,16}$	263 326.775	130.7	10.28	†			
tEME-EE'	$21_{6,16}$–$21_{5,17}$	263 327.628	130.7	10.29	263 327.4	0.51	0.14	HC_3N $v_7 = 1$,CH_3COCH_3
tEME-EE	$21_{6,16}$–$21_{5,17}$	263 327.697	130.7	10.27	†			
tEME-EA	$21_{6,16}$–$21_{5,16}$	263 327.838	130.7	.64	†			
tEME-AE	$21_{6,16}$–$21_{5,17}$	263 328.113	130.7	10.28	†			
tEME-EA	$21_{6,15}$–$21_{5,16}$	263 329.805	130.7	9.67	263 329.9	0.74	0.30	HC_3N $v_7 = 1$,CH_3COCH_3
tEME-AA	$21_{6,15}$–$21_{5,16}$	263 329.839	130.7	10.31	†			
tEME-EA	$21_{6,16}$–$21_{5,17}$	263 330.025	130.7	9.67	†			
tEME-AA	$21_{6,16}$–$21_{5,17}$	263 330.894	130.7	10.31	†			
tEME-EE	$20_{6,14}$–$20_{5,15}$	263 370.802	122.6	9.73	263 370.7	0.51	0.16	$SO^{18}O$, CH_3OCOH
tEME-EE'	$20_{6,14}$–$20_{5,15}$	263 370.865	122.6	9.74	†			
tEME-AE	$20_{6,14}$–$20_{5,15}$	263 371.289	122.6	9.73	†			
tEME-EE'	$20_{6,15}$–$20_{5,16}$	263 372.112	122.6	9.74	263 372.2	0.37	0.16	$SO^{18}O$, CH_3OCOH
tEME-EE	$20_{6,15}$–$20_{5,16}$	263 372.174	122.6	9.73	†			
tEME-AE	$20_{6,15}$–$20_{5,16}$	263 372.598	122.6	9.73	†			
tEME-EA	$20_{6,14}$–$20_{5,15}$	263 374.395	122.6	9.49	…	…	0.17	$SO^{18}O$, CH_3OCOH
tEME-EA	$20_{6,15}$–$20_{5,16}$	263 374.447	122.6	9.49	†			
tEME-AA	$20_{6,14}$–$20_{5,15}$	263 374.550	122.6	9.74	†			
tEME-AA	$20_{6,15}$–$20_{5,16}$	263 375.201	122.6	9.74	†			
tEME-EE	$19_{6,13}$–$20_{5,14}$	263 409.117	114.8	9.17	…	…	0.17	CH_3OCH_3

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Species	Transition $J_{K_a,K_c} - J'_{K'_a,K'_c}$	Predicted frequency (MHz)	E_{upp} (K)	S_{ij}	Observed[1] frequency (MHz)	Observed[1] T_{MB} (K)	Model[2] T_{MB} (K)	Blends
tEME-EE'	$19_{6,13}$–$20_{5,14}$	263 409.177	114.8	9.17	†			
tEME-AE	$19_{6,13}$–$20_{5,14}$	263 409.605	114.8	9.17	†			
tEME-EE'	$19_{6,14}$–$20_{5,15}$	263 410.419	114.8	9.17	†			
tEME-EE	$19_{6,14}$–$20_{5,15}$	263 410.479	114.8	9.17	†			
tEME-AE	$19_{6,14}$–$20_{5,15}$	263 410.907	114.8	9.17	†			
tEME-EA	$19_{6,14}$–$20_{5,15}$	263 412.731	114.8	9.09	…	…	0.19	CH_3OCH_3
tEME-EA	$19_{6,13}$–$20_{5,14}$	263 412.749	114.8	9.09	†			
tEME-AA	$19_{6,13}$–$20_{5,14}$	263 413.003	114.8	9.18	†			
tEME-EE	$18_{6,12}$–$18_{5,13}$	263 441.843	107.5	8.61	…	…	0.17	$^{34}SO_2$,$^{33}SO_2$
tEME-EE'	$18_{6,12}$–$18_{5,13}$	263 441.902	107.5	8.61	†			
tEME-AE	$18_{6,12}$–$18_{5,13}$	263 442.334	107.5	8.61	†			
tEME-EE'	$18_{6,13}$–$18_{5,14}$	263 443.145	107.5	8.61	†			
tEME-EE	$18_{6,13}$–$18_{5,14}$	263 443.204	107.5	8.61	†			
tEME-AE	$18_{6,13}$–$18_{5,14}$	263 443.636	107.5	8.61	†			
tEME-EA	$18_{6,13}$–$18_{5,14}$	263 445.453	107.5	8.58	…	…	0.19	$^{34}SO_2$,$^{33}SO_2$
tEME-EA	$18_{6,12}$–$18_{5,13}$	263 445.498	107.5	8.58	†			
tEME-AA	$18_{6,12}$–$18_{5,13}$	263 445.822	107.5	8.61	†			
tEME-AA	$18_{6,13}$–$18_{5,14}$	263 446.051	107.5	8.61	†			
tEME-EE	$17_{6,11}$–$17_{5,12}$	263 469.553	100.5	8.04	263 469.7	0.43	0.17	CH_3CH_2OH
tEME-EE'	$17_{6,11}$–$17_{5,12}$	263 469.612	100.5	8.04	†			
tEME-AE	$17_{6,11}$–$17_{5,12}$	263 470.047	100.5	8.04	†			
tEME-EE'	$17_{6,12}$–$17_{5,13}$	263 470.859	100.5	8.04	†			
tEME-EE	$17_{6,12}$–$17_{5,13}$	263 470.917	100.5	8.04	†			
tEME-AE	$17_{6,12}$–$17_{5,13}$	263 471.352	100.5	8.04	†			
tEME-EA	$17_{6,12}$–$17_{5,13}$	263 473.169	100.5	8.03	263 473.9	0.41	0.19	CH_3CH_2OH
tEME-EA	$17_{6,11}$–$17_{5,12}$	263 473.223	100.5	8.03	†			
tEME-AA	$17_{6,11}$–$17_{5,12}$	263 473.595	100.5	8.04	†			
tEME-AA	$17_{6,12}$–$17_{5,13}$	263 473.725	100.5	8.04	†			
tEME-EE	$16_{6,10}$–$16_{5,11}$	263 492.786	94.0	7.46	263 492.9	0.26	0.17	CH_3OCH_3
tEME-EE'	$16_{6,10}$–$16_{5,11}$	263 492.845	94.0	7.46	†			
tEME-AE	$16_{6,10}$–$16_{5,11}$	263 493.283	94.0	7.46	†			
tEME-EE'	$16_{6,11}$–$16_{5,12}$	263 494.096	94.0	7.46	263 494.2	0.33	0.17	CH_3OCH_3
tEME-EE	$16_{6,11}$–$16_{5,12}$	263 494.155	94.0	7.46	†			
tEME-AE	$16_{6,11}$–$16_{5,12}$	263 494.592	94.0	7.46	†			
tEME-EA	$16_{6,11}$–$16_{5,12}$	263 496.411	94.0	7.46	263 496.6	0.55	0.19	CH_3OCH_3
tEME-EA	$16_{6,10}$–$16_{5,11}$	263 496.468	94.0	7.46	†			
tEME-AA	$16_{6,10}$–$16_{5,11}$	263 496.871	94.0	7.46	†			
tEME-AA	$16_{6,11}$–$16_{5,12}$	263 496.942	94.0	7.46	†			
tEME-EE	$15_{6,9}$–$15_{5,10}$	263 512.049	87.8	6.89	…	…	0.17	CH_3OCH_3
tEME-EE'	$15_{6,9}$–$15_{5,10}$	263 512.108	87.8	6.89	†			
tEME-AE	$15_{6,9}$–$15_{5,10}$	263 512.548	87.8	6.89	†			

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Species	Transition $J_{K_a,K_c} - J'_{K'_a,K'_c}$	Predicted frequency (MHz)	E_{upp} (K)	S_{ij}	Observed[1] frequency (MHz)	Observed[1] T_{MB} (K)	Model[2] T_{MB} (K)	Blends
tEME-EE’	$15_{6,10}$–$15_{5,11}$	263 513.363	87.8	6.89	…	…	0.17	CH_3OCH_3
tEME-EE	$15_{6,10}$–$15_{5,11}$	263 513.422	87.8	6.89	†			
tEME-AE	$15_{6,10}$–$15_{5,10}$	263 513.862	87.8	6.89	†			
tEME-EA	$15_{6,10}$–$15_{5,11}$	263 515.683	87.8	6.88	…	…	0.19	CH_3CH_2CN
tEME-EA	$15_{6,9}$–$15_{5,10}$	263 515.742	87.8	6.88	†			
tEME-AA	$15_{6,9}$–$15_{5,10}$	263 516.163	87.8	6.89	†			
tEME-AA	$15_{6,10}$–$15_{5,11}$	263 516.200	87.8	6.89	†			
tEME-EE	$14_{6,8}$–$14_{5,9}$	263 527.818	82.0	6.30	…	…	0.16	CH_3OCH_3, CH_3CH_2CN
tEME-EE’	$14_{6,8}$–$14_{5,9}$	263 527.877	82.0	6.30	†			
tEME-AE	$14_{6,8}$–$14_{5,9}$	263 528.319	82.0	6.30	†			
tEME-EE’	$14_{6,9}$–$14_{5,10}$	263 529.136	82.0	6.30	†			
tEME-EE	$14_{6,9}$–$14_{5,10}$	263 529.195	82.0	6.30	†			
tEME-AE	$14_{6,9}$–$14_{5,10}$	263 529.637	82.0	6.30	†			
tEME-EA	$14_{6,9}$–$14_{5,10}$	263 531.461	82.0	6.30	…	…	0.18	CH_3OCH_3
tEME-EA	$14_{6,8}$–$14_{5,9}$	263 531.520	82.0	6.30	†			
tEME-AA	$14_{6,8}$–$14_{5,9}$	263 531.953	82.0	6.30	†			
tEME-AA	$14_{6,9}$–$14_{5,10}$	263 531.971	82.0	6.30	†			
tEME-EE	$13_{6,7}$–$13_{5,8}$	263 540.536	76.6	5.71	…	…	0.15	NH_2CHO, SO_2
tEME-EE’	$13_{6,7}$–$13_{5,8}$	263 540.595	76.6	5.71	†			
tEME-AE	$13_{6,7}$–$13_{5,8}$	263 541.040	76.6	5.71	†			
tEME-EE’	$13_{6,8}$–$13_{5,9}$	263 541.858	76.6	5.71	†			
tEME-EE	$13_{6,8}$–$13_{5,9}$	263 541.917	76.6	5.71	†			
tEME-AE	$13_{6,8}$–$13_{5,9}$	263 542.362	76.6	5.71	†			
tEME-EA	$13_{6,8}$–$13_{5,9}$	263 544.188	76.6	5.71	…	…	0.18	NH_2CHO, SO_2
tEME-EA	$13_{6,7}$–$13_{5,8}$	263 544.247	76.6	5.71	†			
tEME-AA	$13_{6,7}$–$13_{5,8}$	263 544.687	76.6	5.71	†			
tEME-AA	$13_{6,8}$–$13_{5,9}$	263 544.696	76.6	5.71	†			
tEME-EE	$12_{6,6}$–$12_{5,7}$	263 550.619	71.5	5.11	…	…	0.14	SO_2
tEME-EE’	$12_{6,6}$–$12_{5,7}$	263 550.679	71.5	5.11	†			
tEME-AE	$12_{6,6}$–$12_{5,7}$	263 551.125	71.5	5.11	†			
tEME-EE’	$12_{6,7}$–$12_{5,8}$	263 551.945	71.5	5.11	†			
tEME-EE	$12_{6,7}$–$12_{5,8}$	263 552.004	71.5	5.11	†			
tEME-AE	$12_{6,7}$–$12_{5,8}$	263 552.451	71.5	5.11	†			
tEME-EA	$12_{6,7}$–$12_{5,8}$	263 554.279	71.5	5.11	…	…	0.16	SO_2
tEME-EA	$12_{6,6}$–$12_{5,7}$	263 554.338	71.5	5.11	†			
tEME-AA	$12_{6,6}$–$12_{5,7}$	263 554.783	71.5	5.11	†			
tEME-AA	$12_{6,7}$–$12_{5,8}$	263 554.787	71.5	5.11	†			
tEME-EE	$11_{6,5}$–$11_{5,6}$	263 558.451	66.9	4.49	…	…	0.13	SO_2
tEME-EE’	$11_{6,5}$–$11_{5,6}$	263 558.511	66.9	4.49	†			
tEME-AE	$11_{6,5}$–$11_{5,6}$	263 558.959	66.9	4.49	†			
tEME-EE’	$11_{6,6}$–$11_{5,7}$	263 559.780	66.9	4.49	…	…	0.13	SO_2

Species	Transition $J_{K_a,K_c}-J'_{K'_a,K'_c}$	Predicted frequency (MHz)	E_{upp} (K)	S_{ij}	Observed[1] frequency (MHz)	Observed[1] T_{MB} (K)	Model[2] T_{MB} (K)	Blends
tEME-EE	$11_{6,6}$–$11_{5,7}$	263 559.839	66.9	4.49	†			
tEME-AE	$11_{6,6}$–$11_{5,7}$	263 560.288	66.9	4.49	†			
tEME-EA	$11_{6,6}$–$11_{5,7}$	263 562.118	66.9	4.49	…	…	0.15	SO_2
tEME-EA	$11_{6,5}$–$H_{5,6}$	263 562.178	66.9	4.49	†			
tEME-AA	$11_{6,5}$–$11_{5,6}$	263 562.626	66.9	4.49	†			
tEME-AA	$11_{6,6}$–$11_{5,7}$	263 562.627	66.9	4.49	†			
tEME-EE	$10_{6,4}$–$10_{5,5}$	263 564.386	62.7	3.85	…	…	0.11	SO_2
tEME-EE'	$10_{6,4}$–$10_{5,5}$	263 564.446	62.7	3.85	†			
tEME-AE	$10_{6,4}$–$10_{5,5}$	263 564.897	62.7	3.85	†			
tEME-EE'	$10_{6,5}$–$10_{5,6}$	263 565.718	62.7	3.85	…	…	0.11	SO_2
tEME-EE	$10_{6,5}$–$10_{5,6}$	263 565.777	62.7	3.85	†			
tEME-AE	$10_{6,5}$–$10_{5,6}$	263 566.228	62.7	3.85	†			
tEME-EA	$10_{6,5}$–$10_{5,6}$	263 568.061	62.7	3.85	…	…	0.21	SO_2
tEME-EA	$10_{6,4}$–$10_{5,5}$	263 568.120	62.7	3.85	†			
tEME-AA	$10_{6,4}$–$10_{5,5}$	263 568.570	62.7	3.85	†			
tEME-AA	$10_{6,5}$–$10_{5,6}$	263 568.571	62.7	3.85	†			
tEME-EE	$9_{6,3}$–$9_{5,4}$	263 568.750	58.8	3.19	†			
tEME-EE'	$9_{6,3}$–$9_{5,4}$	263 568.810	58.8	3.19	†			
tEME-AE	$9_{6,3}$–$9_{5,4}$	263 569.262	58.8	3.19	†			
tEME-EE'	$9_{6,4}$–$9_{5,5}$	263 570.083	58.8	3.19	†			
tEME-EE	$9_{6,4}$–$9_{5,5}$	263 570.143	58.8	3.19	†			
tEME-AE	$9_{6,4}$–$9_{5,5}$	263 570.595	58.8	3.19	†			
tEME-AE	$8_{6,2}$–$8_{5,3}$	263 572.350	55.3	2.50	263 572.9	0.47	0.20	CH_3OCH_3, HNCO
tEME-EA	$9_{6,4}$–$9_{5,5}$	263 572.430	58.8	3.19	†			
tEME-EA	$9_{6,3}$–$9_{5,4}$	263 572.490	58.8	3.19	†			
tEME-AA	$9_{6,3}$–$9_{5,4}$	263 572.942	58.8	3.19	†			
tEME-AA	$9_{6,4}$–$9_{5,5}$	263 572.942	58.8	3.19	†			
tEME-EE'	$8_{6,3}$–$8_{5,4}$	263 573.172	55.3	2.50	†			
tEME-EE	$8_{6,3}$–$8_{5,4}$	263 573.232	55.3	2.50	†			
tEME-AE	$8_{6,3}$–$8_{5,4}$	263 573.685	55.3	2.50	†			
tEME-EE	$7_{6,1}$–$7_{5,2}$	263 573.911	52.2	1.75	†			
tEME-EE'	$7_{6,1}$–$7_{5,2}$	263 573.972	52.2	1.75	†			
tEME-AE	$7_{6,1}$–$7_{5,2}$	263 574.426	52.2	1.75	†			
tEME-EE	$6_{6,0}$–$6_{5,1}$	263 575.211	49.5	0.93	…	…	0.17	CH_3OCH_3, HNCO
tEME-EE'	$7_{6,2}$–$7_{5,3}$	263 575.249	52.2	1.75	†			
tEME-EE'	$6_{6,0}$–$6_{5,1}$	263 575.271	49.5	0.93	†			
tEME-EE	$7_{6,2}$–$7_{5,3}$	263 575.309	52.2	1.75	†			
tEME-EA	$8_{6,3}$–$8_{5,4}$	263 575.522	55.3	2.50	†			
tEME-EA	$8_{6,2}$–$8_{5,3}$	263 575.582	55.3	2.50	†			
tEME-AE	$6_{6,0}$–$6_{5,1}$	263 575.727	49.5	0.93	†			
tEME-AE	$7_{6,2}$–$7_{5,3}$	263 575.764	52.2	1.75	†			

Species	Transition $J_{K_a,K_c} - J'_{K'_a,K'_c}$	Predicted frequency (MHz)	E_{upp} (K)	S_{ij}	Observed[1] frequency (MHz)	Observed[1] T_{MB} (K)	Model[2] T_{MB} (K)	Blends
tEME-AE	$6_{6,1}$–$6_{5,2}$	263 577.066	49.5	0.93	…	…	0.08	CH_3OCH_3, HNCO
tEME-EA	$7_{6,2}$–$7_{5,3}$	263 577.602	52.2	1.75	†			
tEME-EA	$7_{6,1}$–$7_{5,2}$	263 577.662	52.2	1.75	†			
tEME-AA	$7_{6,1}$–$7_{5,2}$	263 578.117	52.2	1.75	†			
tEME-AA	$7_{6,2}$–$7_{5,3}$	263 578.117	52.2	1.75	†			
tEME-EA	$6_{6,1}$–$6_{5,2}$	263 578.906	49.5	0.93	†			
tEME-EA	$6_{6,0}$–$6_{5,1}$	263 578.966	49.5	0.93	†			
tEME-AA	$6_{6,0}$–$6_{5,1}$	263 579.422	49.5	0.93	†			
tEME-AA	$6_{6,1}$–$6_{5,2}$	263 579.422	49.5	0.93	†			
tEME-EE	$6_{5,1}$–$5_{4,1}$	263 974.290	36.9	4.57	263 974.6	0.84	0.32	CH_3CH_2CN v_{20} = 1, $CH_3{}^{13}CH_2CN$
tEME-EE’	$6_{5,2}$–$5_{4,2}$	263 974.352	36.9	4.57	†			
tEME-EE’	$6_{5,1}$–$5_{4,1}$	263 974.491	36.9	4.57	†			
tEME-EE	$6_{5,2}$–$5_{4,2}$	263 974.554	36.9	4.57	†			
tEME-AE	$6_{5,1}$–$5_{4,1}$	263 974.847	36.9	4.57	†			
tEME-AE	$6_{5,2}$–$5_{4,2}$	263 974.909	36.9	4.57	†			
tEME-EA	$6_{5,2}$–$5_{4,2}$	263 977.560	36.9	4.57	263 977.9	1.19	0.21	CH_3CH_2CN v_{20} = 1,$CH_3{}^{13}CH_2CN$, CH_3OCOH v_t = 1
tEME-EA	$6_{5,1}$–$5_{4,1}$	263 977.761	36.9	4.57	†			
tEME-AA	$6_{5,2}$–$5_{4,1}$	263 978.116	36.9	4.57	†			
tEME-AA	$6_{5,1}$–$5_{4,2}$	263 978.117	36.9	4.57	†			
tEME-EE’	$12_{4,9}$–$11_{3,8}$	264 279.974	48.6	1.86	…	…	0.04	CH_3CH_2CN v_{13}/v_{21}
tEME-AE	$12_{4,9}$–$11_{3,8}$	264 281.470	48.6	1.98	†			
tEME-EE	$12_{4,8}$–$11_{3,8}$	264 282.160	48.6	2.11	†			
tEME-EA	$12_{4,9}$–$11_{3,8}$	264 288.936	48.6	3.18	264 290.1	0.32	0.08	CH_3CH_2CN v_{13}/v_{21}
tEME-AA	$12_{4,9}$–$11_{3,8}$	264 289.975	48.6	4.89	†			
tEME-EE	$12_{4,8}$–$11_{3,8}$	264 290.781	48.6	2.78	†			
tEME-EA	$12_{4,8}$–$11_{3,8}$	264 290.868	48.6	1.70	†			
tEME-AE	$12_{4,8}$–$11_{3,8}$	264 291.901	48.6	2.91	264 292.2	0.33	0.07	CH_3CH_2CN v_{13}/v_{21}
tEME-EE’	$12_{4,8}$–$11_{3,8}$	264 292.217	48.6	3.02	†			
tEME-EE’	$12_{4,9}$–$11_{3,9}$	264 316.948	48.6	3.02	…	…	0.06	CH_3OH
tEME-AE	$12_{4,9}$–$11_{3,9}$	264 318.041	48.6	2.91	†			
tEME-EE	$12_{4,9}$–$11_{3,9}$	264 318.385	48.6	2.78	†			
tEME-EA	$12_{4,9}$–$11_{3,9}$	264 324.363	48.6	1.70	…	…	0.10	CH_3OH
tEME-AA	$12_{4,8}$–$11_{3,9}$	264 326.032	48.6	4.89	†			
tEME-EA	$12_{4,8}$–$11_{3,9}$	264 326.294	48.6	3.18	†			
tEME-EE	$12_{4,8}$–$11_{3,9}$	264 327.005	48.6	2.11	†			
tEME-AE	$12_{4,8}$–$11_{3,9}$	264 328.472	48.6	1.98	…	…	0.04	CH_3OH
tEME-EE’	$12_{4,8}$–$11_{3,9}$	264 329.191	48.6	1.86	†			
tEME-EE’	$30_{2,29}$–$29_{1,28}$	264 623.050	183.6	14.10	…	…	0.14	CH_3CH_2CN v_{13}/v_{21}
tEME-EE	$30_{2,29}$–$29_{1,28}$	264 623.050	183.6	14.10	†			

Species	Transition $J_{K_a,K_c} - J'_{K'_a,K'_c}$	Predicted frequency (MHz)	E_{upp} (K)	S_{ij}	Observed[1] frequency (MHz)	Observed[1] T_{MB} (K)	Model[2] T_{MB} (K)	Blends
tEME-AE	$30_{2,29}$–$29_{1,28}$	264 623.125	183.6	14.10	†			
tEME-EA	$30_{2,29}$–$29_{1,28}$	264 624.097	183.6	14.10	†			
tEME-AA	$30_{2,29}$–$29_{1,28}$	264 624.172	183.6	14.10	†			
tEME-AA	$35_{1,34}$–$34_{2,33}$	265 627.614	246.2	18.59	…	…	0.13	CH_3COOCH_3
tEME-EA	$35_{1,34}$–$34_{2,33}$	265 627.630	246.2	18.59	†			
tEME-AE	$35_{1,34}$–$34_{2,33}$	265 628.218	246.2	18.59	†			
tEME-EE	$35_{1,34}$–$34_{2,33}$	265 628.234	246.2	18.59	†			
tEME-EE’	$35_{1,34}$–$34_{2,33}$	265 628.234	246.2	18.59	†			
tEME-EE’	$19_{3,17}$–$18_{2,16}$	265 859.733	83.8	5.59	…	…	0.13	HCN
tEME-EE	$19_{3,17}$–$18_{2,16}$	265 859.748	83.8	5.59	†			
tEME-AE	$19_{3,17}$–$18_{2,16}$	265 860.022	83.8	5.59	†			
tEME-EA	$19_{3,17}$–$18_{2,16}$	265 862.261	83.8	5.59	…	…	0.09	HCN
tEME-AA	$19_{3,17}$–$18_{2,16}$	265 862.543	83.8	5.59	†			
tEME-EA	$34_{0,34}$–$33_{1,33}$	266 065.053	226.0	28.77	…	…	0.28	CH_3COCH_3
tEME-AA	$34_{0,34}$–$33_{1,33}$	266 065.056	226.0	28.77	†			
tEME-EE	$34_{0,34}$–$33_{1,33}$	266 065.087	226.0	28.77	†			
tEME-EE’	$34_{0,34}$–$33_{1,33}$	266 065.087	226.0	28.77	†			
tEME-AE	$34_{0,34}$–$33_{1,33}$	266 065.091	226.0	28.77	†			
tEME-EE	$18_{3,15}$–$17_{2,16}$	267 851.372	76.5	5.09	267 851.6	0.71	0.13	CH_3OCOH $v_t = 2$
tEME-EE’	$18_{3,15}$–$17_{2,16}$	267 851.394	76.5	5.09	†			
tEME-AE	$18_{3,15}$–$17_{2,16}$	267 851.682	76.5	5.09	†			
tEME-EA	$18_{3,15}$–$17_{2,16}$	267 853.764	76.5	5.09	…	…	0.09	CH_3OCOH $v_t = 2$
tEME-AA	$18_{3,15}$–$17_{2,16}$	267 854.063	76.5	5.09	†			
tEME-EE’	$34_{1,34}$–$33_{0,33}$	267 994.638	226.1	28.78	267 994.7	0.95	0.28	CH_3OCOH $v_t = 2$, CH_3CH_2CN
tEME-EE	$34_{1,34}$–$33_{0,33}$	267 994.638	226.1	28.78	†			
tEME-AE	$34_{1,34}$–$33_{0,33}$	267 994.646	226.1	28.78	†			
tEME-EA	$34_{1,34}$–$33_{0,33}$	267 994.729	226.1	28.78	†			
tEME-AA	$34_{1,34}$–$33_{0,33}$	267 994.737	226.1	28.78	†			
tEME-EE’	$31_{2,30}$–$30_{1,29}$	270 379.929	195.5	14.99	270 380.3	0.21	0.15	
tEME-EE	$31_{2,30}$–$30_{1,29}$	270 379.929	195.5	14.99	†			
tEME-AE	$31_{2,30}$–$30_{1,29}$	270 379.998	195.5	14.99	†			
tEME-EA	$31_{2,30}$–$30_{1,29}$	270 380.924	195.5	14.99	†			
tEME-AA	$31_{2,30}$–$30_{1,29}$	270 380.993	195.5	14.99	†			
tEME-EE	$7_{5,2}$–$6_{4,2}$	272 025.103	39.6	4.70	272 025.5	1.10	0.35	CH_3CH_2CN v_{13}/v_{21}
tEME-EE’	$7_{5,3}$–$6_{4,3}$	272 025.167	39.6	4.70	†			
tEME-EE’	$7_{5,2}$–$6_{4,2}$	272 025.304	39.6	4.70	†			
tEME-EE	$7_{5,3}$–$6_{4,3}$	272 025.368	39.6	4.70	†			
tEME-AE	$7_{5,2}$–$6_{4,2}$	272 025.659	39.6	4.70	†			
tEME-AE	$7_{5,3}$–$6_{4,3}$	272 025.723	39.6	4.70	†			
tEME-EA	$7_{5,3}$–$6_{4,3}$	272 028.370	39.6	4.70	272 028.6	0.59	0.23	CH_3CH_2CN v_{13}/v_{21}

Species	Transition $J_{K_a,K_c} - J'_{K'_a,K'_c}$	Predicted frequency (MHz)	E_{upp} (K)	S_{ij}	Observed[1] frequency (MHz)	Observed[1] T_{MB} (K)	Model[2] T_{MB} (K)	Blends
tEME-EA	$7_{5,2}$–$6_{4,2}$	272 028.571	39.6	4.70	†			
tEME-AA	$7_{5,3}$–$6_{4,2}$	272 028.925	39.6	4.70	†			
tEME-AA	$7_{5,2}$–$6_{4,3}$	272 028.927	39.6	4.70	†			
tEME-EE’	$13_{4,10}$–$12_{3,9}$	272 291.842	53.6	2.35	272 292.1	0.21	0.03	U-line
tEME-AE	$13_{4,10}$–$12_{3,9}$	272 293.250	53.6	2.46	272 293.6	0.26	0.05	U-line
tEME-EE	$13_{4,10}$–$12_{3,9}$	272 293.863	53.6	2.58	†			
tEME-EA	$13_{4,10}$–$12_{3,9}$	272 300.368	53.6	3.94	272 301.0	0.18	0.08	CH_3OCOH
tEME-AA	$13_{4,10}$–$12_{3,9}$	272 301.238	53.6	5.09	†			
tEME-EE	$13_{4,9}$–$12_{3,9}$	272 302.533	53.6	2.51	†			
tEME-EA	$13_{4,9}$–$12_{3,9}$	272 302.564	53.6	1.15	†			
tEME-AE	$13_{4,9}$–$12_{3,9}$	272 303.710	53.6	2.64	272 303.9	0.24	0.07	CH_3CH_2CN $v_{20} = 1$
tEME-EE’	$13_{4,9}$–$12_{3,9}$	272 304.098	53.6	2.74	†			
tEME-EE’	$13_{4,10}$–$12_{3,10}$	272 351.722	53.6	2.74	…	…	0.06	CH_3OH, CH_3OD
tEME-AE	$13_{4,10}$–$12_{3,10}$	272 352.884	53.6	2.63	†			
tEME-EE	$13_{4,10}$–$12_{3,10}$	272 353.288	53.6	2.51	†			
tEME-EA	$13_{4,10}$–$12_{3,10}$	272 359.310	53.6	1.15	…	…	0.13	CH_3OH, CH_3OD
tEME-AA	$13_{4,9}$–$12_{3,10}$	272 361.410	53.6	5.09	†			
tEME-EA	$13_{4,9}$–$12_{3,10}$	272 361.506	53.6	3.94	†			
tEME-EE	$13_{4,9}$–$12_{3,10}$	272 361.957	53.6	2.58	†			
tEME-AE	$13_{4,9}$–$12_{3,10}$	272 363.344	53.6	2.46	…	…	0.05	CH_3OH, CH_3OD
tEME-EE’	$13_{4,9}$–$12_{3,10}$	272 363.978	53.6	2.35	†			
tEME-EE’	$20_{3,18}$–$19_{2,17}$	272 432.754	91.6	5.79	272 433.0	0.33	0.14	U-line
tEME-EE	$20_{3,18}$–$19_{2,17}$	272 432.765	91.6	5.79	†			
tEME-AE	$20_{3,18}$–$19_{2,17}$	272 433.037	91.6	5.79	†			
tEME-EA	$20_{3,18}$–$19_{2,17}$	272 435.273	91.6	5.79	272 435.7	0.35	0.09	U-line
tEME-AA	$20_{3,18}$–$19_{2,17}$	272 435.550	91.6	5.79	†			
tEME-AA	$40_{2,38}$–$39_{3,37}$	272 596.983	325.0	12.66	…	…	0.03	U-line
tEME-EA	$40_{2,38}$–$39_{3,37}$	272 597.055	325.0	12.66	†			
tEME-AE	$40_{2,38}$–$39_{3,37}$	272 598.688	325.0	12.66	†			
tEME-EE	$40_{2,38}$–$39_{3,37}$	272 598.760	325.0	12.66	†			
tEME-EE’	$40_{2,38}$–$39_{3,37}$	272 598.760	325.0	12.66	†			
tEME-EE	$20_{2,18}$–$19_{1,19}$	273 141.137	86.3	2.00	…	…	0.05	CH_3OCOH
tEME-EE’	$20_{2,18}$–$19_{1,19}$	273 141.138	86.3	2.00	†			
tEME-AE	$20_{2,18}$–$19_{1,19}$	273 141.411	86.3	2.00	†			
tEME-EA	$20_{2,18}$–$19_{1,19}$	273 142.818	86.3	2.00	…	…	0.03	CH_3OCOH
tEME-AA	$20_{2,18}$–$19_{1,19}$	273 143.092	86.3	2.00	†			
tEME-EA	$35_{0,35}$–$34_{1,34}$	273 979.063	239.2	29.79	273 979.1	0.73	0.28	CH_3CH_2CN, SO_2
tEME-AA	$35_{0,35}$–$34_{1,34}$	273 979.067	239.2	29.79	†			
tEME-EE	$35_{0,35}$–$34_{1,34}$	273 979.089	239.2	29.79	†			
tEME-EE’	$35_{0,35}$–$34_{1,34}$	273 979.089	239.2	29.79	†			
tEME-AE	$35_{0,35}$–$34_{1,34}$	273 979.093	239.2	29.79	†			

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tEME-AA	$36_{1,35}$–$35_{2,34}$	274 946.543	260.0	19.65	274 946.9	0.57	0.14	CH_3OCOH v_t = 1, H_2CS
tEME-EA	$36_{1,35}$–$35_{2,34}$	274 946.555	260.0	19.65	†			
tEME-AE	$36_{1,35}$–$35_{2,34}$	274 947.090	260.0	19.65	†			
tEME-EE	$36_{1,35}$–$35_{2,34}$	274 947.102	260.0	19.65	†			
tEME-EE’	$36_{1,35}$–$35_{2,34}$	274 947.102	260.0	19.65	†			
tEME-EE’	$35_{1,35}$–$34_{0,34}$	275 618.927	239.3	29.80	275 618.9	0.22	0.28	
tEME-EE	$35_{1,35}$–$34_{0,34}$	275 618.927	239.3	29.80	†			
tEME-AE	$35_{1,35}$–$34_{0,34}$	275 618.934	239.3	29.80	†			
tEME-EA	$35_{1,35}$–$34_{0,34}$	275 619.009	239.3	29.80	†			
tEME-AA	$35_{1,35}$–$34_{0,34}$	275 619.016	239.3	29.80	†			
tEME-EE’	$32_{2,31}$–$31_{1,30}$	276 219.631	207.8	15.92	276 219.6	0.34	0.15	$^{13}CH_3OCOH$
tEME-EE	$32_{2,31}$–$31_{1,30}$	276 219.631	207.8	15.92	†			
tEME-AE	$32_{2,31}$–$31_{1,30}$	276 219.695	207.8	15.92	†			
tEME-EA	$32_{2,31}$–$31_{1,30}$	276 220.573	207.8	15.92	†			
tEME-AA	$32_{2,31}$–$31_{1,30}$	276 220.637	207.8	15.92	†			
tEME-EE	$19_{3,16}$–$18_{2,17}$	276 700.152	83.9	5.20	276 700.3	0.29	0.13	CH_3CN v_8 = 1, CH_3OH
tEME-EE’	$19_{3,16}$–$18_{2,17}$	276 700.167	83.9	5.20	†			
tEME-AE	$19_{3,16}$–$18_{2,17}$	276 700.458	83.9	5.20	†			
tEME-EA	$19_{3,16}$–$18_{2,17}$	276 702.533	83.9	5.20	276 702.5	0.34	0.08	CH_3CN v_8 = 1, CH_3OH
tEME-AA	$19_{3,16}$–$18_{2,17}$	276 702.832	83.9	5.20	†			
tEME-EE’	$21_{3,19}$–$20_{2,18}$	278 825.580	99.7	6.00	278 825.7	0.39	0.14	CH_3CH_2CN, CH_3CH_2CN v_{20} = 1, $CH_3{}^{13}CH_2CN$
tEME-EE	$21_{3,19}$–$20_{2,18}$	278 825.588	99.7	6.00	†			
tEME-AE	$21_{3,19}$–$20_{2,18}$	278 825.856	99.7	6.00	†			
tEME-EA	$21_{3,19}$–$20_{2,18}$	278 828.090	99.7	6.00	278 828.4	0.33	0.09	CH_3CH_2CN, CH_3CH_2CN v_{20} = 1, $CH_3{}^{13}CH_2CN$
tEME-AA	$21_{3,19}$–$20_{2,18}$	278 828.362	99.7	6.00	†			
tEME-EE	$8_{5,3}$–$7_{4,3}$	280 075.262	42.7	4.85	280 075.6	0.40	0.38	
tEME-EE’	$8_{5,4}$–$7_{4,4}$	280 075.328	42.7	4.85	†			
tEME-EE’	$8_{5,3}$–$7_{4,3}$	280 075.462	42.7	4.85	†			
tEME-EE	$8_{5,4}$–$7_{4,4}$	280 075.527	42.7	4.85	†			
tEME-AE	$8_{5,3}$–$7_{4,3}$	280 075.816	42.7	4.85	†			
tEME-AE	$8_{5,4}$–$7_{4,4}$	280 075.882	42.7	4.85	†			
tEME-EA	$8_{5,4}$–$7_{4,4}$	280 078.526	42.7	4.85	280 078.5	0.31	0.25	
tEME-EA	$8_{5,3}$–$7_{4,3}$	280 078.726	42.7	4.85	†			
tEME-AA	$8_{5,4}$–$7_{4,3}$	280 079.076	42.7	4.85	†			
tEME-AA	$8_{5,3}$–$7_{4,4}$	280 079.084	42.7	4.85	†			
tEME-EE’	$14_{4,11}$–$13_{3,10}$	280 288.955	59.0	2.84	…	…	0.07	CH_3COOH v_t = 1
tEME-AE	$14_{4,11}$–$13_{3,10}$	280 290.299	59.0	2.96	†			
tEME-EE	$14_{4,11}$–$13_{3,10}$	280 290.853	59.0	3.11	†			
tEME-EA	$14_{4,11}$–$13_{3,10}$	280 297.013	59.0	4.69	280 297.7	0.12	0.10	
tEME-AA	$14_{4,11}$–$13_{3,10}$	280 297.720	59.0	5.30	†			

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Species	Transition $J_{K_a,K_c} - J'_{K'_a,K'_c}$	Predicted frequency (MHz)	E_{upp} (K)	S_{ij}	Observed[1] frequency (MHz)	Observed[1] T_{MB} (K)	Model[2] T_{MB} (K)	Blends
tEME-EE	$14_{4,10}$–$13_{3,10}$	280 299.704	59.0	2.19	280 301.1	0.10	0.06	U-line
tEME-EA	$14_{4,10}$–$13_{3,10}$	280 299.889	59.0	0.61	†			
tEME-AE	$14_{4,10}$–$13_{3,10}$	280 300.898	59.0	2.34	†			
tEME-EE’	$14_{4,10}$–$13_{3,10}$	280 301.316	59.0	2.46	†			
tEME-EE’	$14_{4,11}$–$13_{3,11}$	280 383.694	59.0	2.46	280 385.0	0.11	0.06	CH_3OCOH $v_t = 1$
tEME-AE	$14_{4,11}$–$13_{3,11}$	280 384.884	59.0	2.34	†			
tEME-EE	$14_{4,11}$–$13_{3,11}$	280 385.307	59.0	2.19	†			
tEME-EA	$14_{4,10}$–$13_{3,11}$	280 394.040	59.0	4.69	…	…	0.16	CH_3OCOH
tEME-AA	$14_{4,10}$–$13_{3,11}$	280 394.104	59.0	5.30	†			
tEME-EE	$14_{4,10}$–$13_{3,11}$	280 394.157	59.0	3.11	†			
tEME-AE	$14_{4,10}$–$13_{3,11}$	280 395.482	59.0	2.96	†			
tEME-EE’	$14_{4,10}$–$13_{3,11}$	280 396.055	59.0	2.83	†			
tEME-EA	$36_{0,36}$–$35_{1,35}$	281 871.802	252.8	30.81	281 871.7	0.25	0.27	U-line
tEME-AA	$36_{0,36}$–$35_{1,35}$	281 871.806	252.8	30.81	†			
tEME-EE	$36_{0,36}$–$35_{1,35}$	281 871.822	252.8	30.81	†			
tEME-EE’	$36_{0,36}$–$35_{1,35}$	281 871.822	252.8	30.81	†			
tEME-AE	$36_{0,36}$–$35_{1,35}$	281 871.826	252.8	30.81	†			
tEME-EE’	$33_{2,32}$–$32_{1,31}$	282 152.573	220.4	16.88	282 153.2	0.56	0.16	HC_3N $v_5 = 1$
tEME-EE	$33_{2,32}$–$32_{1,31}$	282 152.573	220.4	16.88	†			
tEME-AE	$33_{2,32}$–$32_{1,31}$	282 152.631	220.4	16.88	†			
tEME-EA	$33_{2,32}$–$32_{1,31}$	282 153.461	220.4	16.88	†			
tEME-AA	$33_{2,32}$–$32_{1,31}$	282 153.519	220.4	16.88	†			
tEME-EE’	$36_{1,36}$–$35_{0,35}$	283 263.283	252.8	30.82	283 263.4	0.44	0.27	$^{13}CH_3OH$
tEME-EE	$36_{1,36}$–$35_{0,35}$	283 263.283	252.8	30.82	†			
tEME-AE	$36_{1,36}$–$35_{0,35}$	283 263.290	252.8	30.82	†			
tEME-EA	$36_{1,36}$–$35_{0,35}$	283 263.357	252.8	30.82	†			
tEME-AA	$36_{1,36}$–$35_{0,35}$	283 263.364	252.8	30.82	†			
tEME-AE	$41_{2,39}$–$40_{3,38}$	283 951.422	341.0	13.47	…	…	0.03	CH_3OCH_3
tEME-EE	$41_{2,39}$–$40_{3,38}$	283 951.485	341.0	13.47	†			
tEME-EE’	$41_{2,39}$–$40_{3,38}$	283 951.485	341.0	13.47	†			
tEME-AA	$37_{1,36}$–$36_{2,35}$	284 137.669	274.2	20.72	288 138.3	0.34	0.14	CH_3OCOH $v_t = 1$
tEME-EA	$37_{1,36}$–$36_{2,35}$	284 137.677	274.2	20.72	†			
tEME-AE	$37_{1,36}$–$36_{2,35}$	284 138.161	274.2	20.72	†			
tEME-EE	$37_{1,36}$–$36_{2,35}$	284 138.169	274.2	20.72	†			
tEME-EE’	$37_{1,36}$–$36_{2,35}$	284 138.169	274.2	20.72	†			
tEME-EE’	$22_{3,20}$–$21_{2,19}$	285 037.438	108.2	6.21	…	…	0.14	CH_3CH_2CN v_{13}/v_{21}
tEME-EE	$22_{3,20}$–$21_{2,19}$	285 037.444	108.2	6.21	†			
tEME-AE	$22_{3,20}$–$21_{2,19}$	285 037.708	108.2	6.21	†			
tEME-EA	$22_{3,20}$–$21_{2,19}$	285 039.939	108.2	6.21	…	…	0.09	CH_3CH_2CN v_{13}/v_{21}
tEME-AA	$22_{3,20}$–$21_{2,19}$	285 040.206	108.2	6.21	†			
tEME-EE	$20_{3,17}$–$19_{2,18}$	285 699.473	91.6	5.28	…	…	0.14	SO_2

Species	Transition $J_{K_a,K_c} - J'_{K'_a,K'_c}$	Predicted frequency (MHz)	E_{upp} (K)	S_{ij}	Observed[1] frequency (MHz)	Observed[1] T_{MB} (K)	Model[2] T_{MB} (K)	Blends
tEME-EE’	$20_{3,17}$–$19_{2,18}$	285 699.484	91.6	5.28	†			
tEME-AE	$20_{3,17}$–$19_{2,18}$	285 699.777	91.6	5.28	†			
tEME-EA	$20_{3,17}$–$19_{2,18}$	285 701.840	91.6	5.28	…	…	0.10	SO_2
tEME-AA	$20_{3,17}$–$19_{2,18}$	285 702.139	91.6	5.28	†			
tEME-EE	$21_{2,19}$–$20_{1,20}$	286 585.825	94.5	1.86	…	…	0.05	CH_3COOH $v_t = 1$
tEME-EE’	$21_{2,19}$–$20_{1,20}$	286 585.825	94.5	1.86	†			
tEME-AE	$21_{2,19}$–$20_{1,20}$	286 586.110	94.5	1.86	†			
tEME-EA	$21_{2,19}$–$20_{1,20}$	286 587.511	94.5	1.86	…	…	0.03	U-line
tEME-AA	$21_{2,19}$–$20_{1,20}$	286 587.796	94.5	1.86	†			
tEME-EE	$9_{5,4}$–$8_{4,4}$	288 124.443	46.1	5.02	288 124.8	0.59	0.41	
tEME-EE’	$9_{5,5}$–$8_{4,5}$	288 124.510	46.1	5.02	†			
tEME-EE’	$9_{5,4}$–$8_{4,4}$	288 124.641	46.1	5.02	†			
tEME-EE	$9_{5,5}$–$8_{4,5}$	288 124.708	46.1	5.02	†			
tEME-AE	$9_{5,4}$–$8_{4,4}$	288 124.995	46.1	5.02	†			
tEME-AE	$9_{5,5}$–$8_{4,5}$	288 125.062	46.1	5.02	†			
tEME-EA	$9_{5,5}$–$8_{4,5}$	288 127.703	46.1	5.02	…	…	0.27	CH_3OCOH
tEME-EA	$9_{5,4}$–$8_{4,4}$	288 127.901	46.1	5.02	†			
tEME-AA	$9_{5,5}$–$8_{4,4}$	288 128.242	46.1	5.02	†			
tEME-AA	$9_{5,4}$–$8_{4,5}$	288 128.268	46.1	5.02	†			
tEME-EE’	$34_{2,33}$–$33_{1,32}$	288 187.160	233.4	17.86	288 187.5	0.54	0.17	CH_3OCOH
tEME-EE	$34_{2,33}$–$33_{1,32}$	288 187.160	233.4	17.86	†			
tEME-AE	$34_{2,33}$–$33_{1,32}$	288 187.214	233.4	17.86	†			
tEME-EA	$34_{2,33}$–$33_{1,32}$	288 187.993	233.4	17.86	†			
tEME-AA	$34_{2,33}$–$33_{1,32}$	288 188.047	233.4	17.86	†			
tEME-EE’	$15_{4,12}$–$14_{3,11}$	288 267.539	64.8	3.40	…	…	0.09	$SO^{18}O$, CH_3COCH_3
tEME-AE	$15_{4,12}$–$14_{3,11}$	288 268.817	64.8	3.55	†			
tEME-EE	$15_{4,12}$–$14_{3,11}$	288 269.302	64.8	3.75	†			
tEME-EA	$15_{4,12}$–$14_{3,11}$	288 274.971	64.8	5.24	288 275.12	0.14	0.12	$SO^{18}O$
tEME-AA	$15_{4,12}$–$14_{3,11}$	288 275.555	64.8	5.50	†			
tEME-EE	$15_{4,11}$–$14_{3,11}$	288 278.681	64.8	1.75	…	…	0.05	U-line
tEME-AE	$15_{4,11}$–$14_{3,11}$	288 279.849	64.8	1.95	†			
tEME-EE’	$15_{4,11}$–$14_{3,11}$	288 280.260	64.8	2.11	†			
tEME-EE’	$15_{4,12}$–$14_{3,12}$	288 413.150	64.8	2.11	…	…	0.05	U-line
tEME-AE	$15_{4,12}$–$14_{3,12}$	288 414.329	64.8	1.95	†			
tEME-EE	$15_{4,12}$–$14_{3,12}$	288 414.729	64.8	1.75	†			
tEME-EE	$15_{4,11}$–$14_{3,12}$	288 424.108	64.8	3.75	288 424.7	0.50	0.20	$CH_3OC^{18}OH$
tEME-EA	$15_{4,11}$–$14_{3,12}$	288 424.469	64.8	5.24	†			
tEME-AA	$15_{4,11}$–$14_{3,12}$	288 424.653	64.8	5.50	†			
tEME-AE	$15_{4,11}$–$14_{3,12}$	288 425.361	64.8	3.55	†			
tEME-EE’	$15_{4,11}$–$14_{3,12}$	288 425.871	64.8	3.40	†			
tEME-EA	$37_{0,37}$–$36_{1,36}$	289 745.973	266.7	31.83	289 745.8	0.49	0.26	U-line

Species	Transition $J_{K_a,K_c} - J'_{K'_a,K'_c}$	Predicted frequency (MHz)	E_{upp} (K)	S_{ij}	Observed[1] frequency (MHz)	Observed[1] T_{MB} (K)	Model[2] T_{MB} (K)	Blends
tEME-AA	$37_{0,37}$–$36_{1,36}$	289 745.977	266.7	31.83	†			
tEME-EE	$37_{0,37}$–$36_{1,36}$	289 745.986	266.7	31.83	†			
tEME-EE’	$37_{0,37}$–$36_{1,36}$	289 745.986	266.7	31.83	†			
tEME-AE	$37_{0,37}$–$36_{1,36}$	289 745.991	266.7	31.83	†			
tEME-EE’	$37_{1,37}$–$36_{0,36}$	290 924.982	266.8	31.83	290 925.0	0.71	0.27	$^{33}SO_2$
tEME-EE	$37_{1,37}$–$36_{0,36}$	290 924.982	266.8	31.83	†			
tEME-AE	$37_{1,37}$–$36_{0,36}$	290 924.989	266.8	31.83	†			
tEME-EA	$37_{1,37}$–$36_{0,36}$	290 925.049	266.8	31.83	†			
tEME-AA	$37_{1,37}$–$36_{0,36}$	290 925.056	266.8	31.83	†			
tEME-AA	$38_{1,37}$–$37_{2,36}$	293 203.620	288.8	21.79	293 203.7	0.28	0.14	
tEME-EA	$38_{1,37}$–$37_{2,36}$	293 203.624	288.8	21.79	†			
tEME-AE	$38_{1,37}$–$37_{2,36}$	293 204.059	288.8	21.79	†			
tEME-EE	$38_{1,37}$–$37_{2,36}$	293 204.064	288.8	21.79	†			
tEME-EE’	$38_{1,37}$–$37_{2,36}$	293 204.064	288.8	21.79	†			
tEME-EE’	$35_{2,34}$–$34_{1,33}$	294 329.625	246.8	18.86	294 330.0	0.28	0.17	
tEME-EE	$35_{2,34}$–$34_{1,33}$	294 329.625	246.8	18.86	†			
tEME-AE	$35_{2,34}$–$34_{1,33}$	294 329.673	246.8	18.86	†			
tEME-EA	$35_{2,34}$–$34_{1,33}$	294 330.403	246.8	18.86	†			
tEME-AA	$35_{2,34}$–$34_{1,33}$	294 330.451	246.8	18.86	†			
tEME-EE	$21_{3,18}$–$20_{2,19}$	294 868.623	99.8	5.34	…	…	0.15	CH_3OCOH
tEME-EE’	$21_{3,18}$–$20_{2,19}$	294 868.631	99.8	5.34	†			
tEME-AE	$21_{3,18}$–$20_{2,19}$	294 868.926	99.8	5.34	†			
tEME-EE	$37_{2,36}$–$36_{2,35}$	294 869.441	274.8	36.86	†			
tEME-EE’	$37_{2,36}$–$36_{2,35}$	294 869.441	274.8	36.86	†			
tEME-AE	$37_{2,36}$–$36_{2,35}$	294 869.456	274.8	36.86	†			
tEME-EA	$37_{2,36}$–$36_{2,35}$	294 869.504	274.8	36.86	†			
tEME-AA	$37_{2,36}$–$36_{2,35}$	294 869.519	274.8	36.86	†			
tEME-EA	$21_{3,18}$–$20_{2,19}$	294 870.971	99.8	5.34	…	…	0.10	CH_3OCOH
tEME-AA	$21_{3,18}$–$20_{2,19}$	294 871.271	99.8	5.34	†			
tEME-AA	$42_{2,40}$–$41_{3,39}$	295 213.922	357.4	14.32	…	…	0.03	CH_3CN $v_8 = 1$
tEME-EA	$42_{2,40}$–$41_{3,39}$	295 213.976	357.4	14.32	†			
tEME-AE	$42_{2,40}$–$41_{3,39}$	295 215.469	357.4	14.32	†			
tEME-EE	$42_{2,40}$–$41_{3,39}$	295 215.522	357.4	14.32	†			
tEME-EE’	$42_{2,40}$–$41_{3,39}$	295 215.522	357.4	14.32	†			
tEME-EE	$10_{5,5}$–$9_{4,5}$	296 172.265	50.0	5.20	…	…	0.45	SO_2
tEME-EE’	$10_{5,6}$–$9_{4,6}$	296 172.333	50.0	5.20	†			
tEME-EE’	$10_{5,5}$–$9_{4,5}$	296 172.462	50.0	5.20	†			
tEME-EE	$10_{5,6}$–$9_{4,6}$	296 172.530	50.0	5.20	†			
tEME-AE	$10_{5,5}$–$9_{4,5}$	296 172.815	50.0	5.20	†			
tEME-AE	$10_{5,6}$–$9_{4,6}$	296 172.884	50.0	5.20	†			
tEME-EA	$10_{5,6}$–$9_{4,6}$	296 175.521	50.0	5.20	…	…	0.30	SO_2

Species	Transition $J_{K_a,K_c} - J'_{K'_a,K'_c}$	Predicted frequency (MHz)	E_{upp} (K)	S_{ij}	Observed[1] frequency (MHz)	Observed[1] T_{MB} (K)	Model[2] T_{MB} (K)	Blends
tEME-EA	$10_{5,5}$–$9_{4,5}$	296 175.717	50.0	5.20	†			
tEME-AA	$10_{5,6}$–$9_{4,5}$	296 176.037	50.0	5.20	†			
tEME-AA	$10_{5,5}$–$9_{4,6}$	296 176.104	50.0	5.20	†			
tEME-EE’	$16_{4,13}$–$15_{3,12}$	296 223.035	71.0	4.07	296 224.2	0.49	0.11	CH_3OCOH
tEME-AE	$16_{4,13}$–$15_{3,12}$	296 224.220	71.0	4.26	†			
tEME-EE	$16_{4,13}$–$15_{3,12}$	296 224.598	71.0	4.49	†			
tEME-EA	$16_{4,13}$–$15_{3,12}$	296 229.670	71.0	5.60	296 230.0	0.30	0.13	CH_3OCOH
tEME-AA	$16_{4,13}$–$15_{3,12}$	296 230.175	71.0	5.70	†			
tEME-EE	$16_{4,12}$–$15_{3,12}$	296 235.284	71.0	1.21	…	…	0.04	CH_3CH_2CN $v_{12} = 1$
tEME-AE	$16_{4,12}$–$15_{3,12}$	296 236.371	71.0	1.44	†			
tEME-EE’	$16_{4,12}$–$15_{3,12}$	296 236.725	71.0	1.63	†			
tEME-EE’	$16_{4,13}$–$15_{3,13}$	296 440.645	71.0	1.63	…	…	0.04	CH_3CH_2CN
tEME-AE	$16_{4,13}$–$15_{3,13}$	296 441.764	71.0	1.44	†			
tEME-EE	$16_{4,13}$–$15_{3,13}$	296 442.086	71.0	1.21	†			
tEME-EE	$16_{4,12}$–$15_{3,13}$	296 452.772	71.0	4.49	…	…	0.24	CH_3CH_2CN
tEME-EA	$16_{4,12}$–$15_{3,13}$	296 453.716	71.0	5.59	†			
tEME-AE	$16_{4,12}$–$15_{3,13}$	296 453.915	71.0	4.26	†			
tEME-AA	$16_{4,12}$–$15_{3,13}$	296 453.976	71.0	5.70	†			
tEME-EE’	$16_{4,12}$–$15_{3,13}$	296 454.335	71.0	4.07	†			
tEME-EE’	$24_{3,22}$–$23_{2,21}$	296 926.193	126.4	6.66	296 926.5	0.17	0.14	
tEME-EE	$24_{3,22}$–$23_{2,21}$	296 926.197	126.4	6.66	†			
tEME-AE	$24_{3,22}$–$23_{2,21}$	296 926.450	126.4	6.66	†			
tEME-EA	$24_{3,22}$–$23_{2,21}$	296 928.675	126.4	6.66	296 928.7	0.42	0.09	CH_3OCOH $v_t = 2$
tEME-AA	$24_{3,22}$–$23_{2,21}$	296 928.931	126.4	6.66	†			
tEME-EA	$38_{0,38}$–$37_{1,37}$	297 603.969	281.1	32.84	…	…	0.25	CH_3OCOH $v_t = 2$
tEME-AA	$38_{0,38}$–$37_{1,37}$	297 603.974	281.1	32.84	†			
tEME-EE	$38_{0,38}$–$37_{1,37}$	297 603.978	281.1	32.84	†			
tEME-EE’	$38_{0,38}$–$37_{1,37}$	297 603.978	281.1	32.84	†			
tEME-AE	$38_{0,38}$–$37_{1,37}$	297 603.982	281.1	32.84	†			
tEME-EE’	$38_{1,38}$–$37_{0,37}$	298 601.597	281.1	32.85	…	…	0.26	SO_2
tEME-EE	$38_{1,38}$–$37_{0,37}$	298 601.597	281.1	32.85	†			
tEME-AE	$38_{1,38}$–$37_{0,37}$	298 601.604	281.1	32.85	†			
tEME-EA	$38_{1,38}$–$37_{0,37}$	298 601.658	281.1	32.85	†			
tEME-AA	$38_{1,38}$–$37_{0,37}$	298 601.665	281.1	32.85	†			
tEME-EE	$22_{2,20}$–$21_{1,21}$	300 442.750	103.1	1.73	…	…	0.05	$H^{13}CCCN$ $v_7 = 1$, CH_3OCOH
tEME-EE’	$22_{2,20}$–$21_{1,21}$	300 442.750	103.1	1.73	†			
tEME-AE	$22_{2,20}$–$21_{1,21}$	300 443.046	103.1	1.73	†			
tEME-EA	$22_{2,20}$–$21_{1,21}$	300 444.445	103.1	1.73	…	…	0.03	$H^{13}CCCN$ $v_7 = 1$, CH_3OCOH
tEME-AA	$22_{2,20}$–$21_{1,21}$	300 444.741	103.1	1.73	†			
tEME-EE’	$36_{2,35}$–$35_{1,34}$	300 583.963	260.6	19.88	300 584.4	0.25	0.17	

Species	Transition $J_{K_a,K_c} - J'_{K'_a,K'_c}$	Predicted frequency (MHz)	E_{upp} (K)	S_{ij}	Observed[1] frequency (MHz)	Observed[1] T_{MB} (K)	Model[2] T_{MB} (K)	Blends
tEME-EE	$36_{2,35}$–$35_{1,34}$	300 583.963	260.6	19.88	†			
tEME-AE	$36_{2,35}$–$35_{1,34}$	300 584.008	260.6	19.88	†			
tEME-EA	$36_{2,35}$–$35_{1,34}$	300 584.687	260.6	19.88	†			
tEME-AA	$36_{2,35}$–$35_{1,34}$	300 584.731	260.6	19.88	†			
tEME-AA	$39_{1,38}$–$38_{2,37}$	302 148.596	303.8	22.87	…	…	0.14	SO_2
tEME-EA	$39_{1,38}$–$38_{2,37}$	302 148.597	303.8	22.87	†			
tEME-AE	$39_{1,38}$–$38_{2,37}$	302 148.985	303.8	22.87	†			
tEME-EE	$39_{1,38}$–$38_{2,37}$	302 148.986	303.8	22.87	†			
tEME-EE’	$39_{1,38}$–$38_{2,37}$	302 148.986	303.8	22.87	†			
tEME-EE’	$25_{3,23}$–$24_{2,22}$	302 611.864	136.1	6.91	…	…	0.14	CH_3COCH_3
tEME-EE	$25_{3,23}$–$24_{2,22}$	302 611.867	136.1	6.91	†			
tEME-AE	$25_{3,23}$–$24_{2,22}$	302 612.114	136.1	6.91	†			
tEME-EA	$25_{3,23}$–$24_{2,22}$	302 614.334	136.1	6.91	…	…	0.09	CH_3COCH_3
tEME-AA	$25_{3,23}$–$24_{2,22}$	302 614.582	136.0	6.91	†			
tEME-EE’	$17_{4,14}$–$16_{3,13}$	304 150.005	77.5	4.81	…	…	0.14	CH_2CHCN
tEME-AE	$17_{4,14}$–$16_{3,13}$	304 151.052	77.5	4.99	†			
tEME-EE	$17_{4,14}$–$16_{3,13}$	304 151.281	77.5	5.19	†			
tEME-EA	$17_{4,14}$–$16_{3,13}$	304 155.769	77.5	5.86	…	…	0.14	CH_2CHCN
tEME-AA	$17_{4,14}$–$16_{3,13}$	304 156.225	77.5	5.90	†			
tEME-EE	$11_{5,6}$–$10_{4,6}$	304 218.289	54.3	5.39	…	…	0.48	CH_3OH
tEME-EE’	$11_{5,7}$–$10_{4,7}$	304 218.360	54.3	5.39	†			
tEME-EE’	$11_{5,6}$–$10_{4,6}$	304 218.485	54.3	5.39	†			
tEME-EE	$11_{5,7}$–$10_{4,7}$	304 218.556	54.3	5.39	†			
tEME-AE	$11_{5,6}$–$10_{4,6}$	304 218.838	54.3	5.39	†			
tEME-AE	$11_{5,7}$–$10_{4,7}$	304 218.909	54.3	5.39	†			
tEME-EA	$11_{5,7}$–$10_{4,7}$	304 221.544	54.3	5.38	…	…	0.32	CH_3OH
tEME-EA	$11_{5,6}$–$10_{4,6}$	304 221.733	54.3	5.38	†			
tEME-AA	$11_{5,7}$–$10_{4,6}$	304 222.011	54.3	5.39	†			
tEME-AA	$11_{5,6}$–$10_{4,7}$	304 222.167	54.3	5.39	†			
tEME-EE	$22_{3,19}$–$21_{2,20}$	304 228.127	108.3	5.38	…	…	0.14	CH_3COCH_3
tEME-EE’	$22_{3,19}$–$21_{2,20}$	304 228.133	108.3	5.38	†			
tEME-AE	$22_{3,19}$–$21_{2,20}$	304 228.430	108.3	5.38	†			
tEME-EA	$22_{3,19}$–$21_{2,20}$	304 230.454	108.3	5.38	…	…	0.10	CH_3COCH_3
tEME-AA	$22_{3,19}$–$21_{2,20}$	304 230.754	108.3	5.38	†			
tEME-EE	$17_{4,13}$–$16_{3,14}$	304 481.623	77.5	5.19	…	…	0.25	CH_3OCOH $v_t = 1$
tEME-AE	$17_{4,13}$–$16_{3,14}$	304 482.613	77.5	4.99	†			
tEME-EE’	$17_{4,13}$–$16_{3,14}$	304 482.900	77.5	4.81	†			
tEME-EA	$17_{4,13}$–$16_{3,14}$	304 483.137	77.5	5.85	†			
tEME-AA	$17_{4,13}$–$16_{3,14}$	304 483.441	77.5	5.90	†			
tEME-EA	$39_{0,39}$–$38_{1,38}$	305 447.899	295.7	33.86	305 448.1	0.96	0.24	CH_3CH_2CN v_{13}/v_{21}
tEME-EE	$39_{0,39}$–$38_{1,38}$	305 447.903	295.7	33.86	†			

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Species	Transition $J_{K_a,K_c} - J'_{K'_a,K'_c}$	Predicted frequency (MHz)	E_{upp} (K)	S_{ij}	Observed[1] frequency (MHz)	Observed[1] T_{MB} (K)	Model[2] T_{MB} (K)	Blends
tEME-EE’	$39_{0,39}$–$38_{1,38}$	305 447.903	295.7	33.86	†			
tEME-AA	$39_{0,39}$–$38_{1,38}$	305 447.904	295.7	33.86	†			
tEME-AE	$39_{0,39}$–$38_{1,38}$	305 447.908	295.7	33.86	†			
tEME-EE	$39_{1,39}$–$38_{0,38}$	306 290.978	295.7	33.86	…	…	0.24	CH_3OH
tEME-EE’	$39_{1,39}$–$38_{0,38}$	306 290.978	295.7	33.86	†			
tEME-AE	$39_{1,39}$–$38_{0,38}$	306 290.985	295.7	33.86	†			
tEME-EA	$39_{1,39}$–$38_{0,38}$	306 291.035	295.7	33.86	†			
tEME-AA	$39_{1,39}$–$38_{0,38}$	306 291.041	295.7	33.86	†			
tEME-AA	$43_{2,41}$–$42_{3,40}$	306 373.059	374.1	15.22	…	…	0.03	CH_3OCH_3
tEME-EA	$43_{2,41}$–$42_{3,40}$	306 373.104	374.1	15.22	†			
tEME-AE	$43_{2,41}$–$42_{3,40}$	306 374.522	374.1	15.22	†			
tEME-EE	$43_{2,41}$–$42_{3,40}$	306 374.567	374.1	15.22	†			
tEME-EE’	$43_{2,41}$–$2_{3,40}$	306 374.567	374.1	15.22	†			

Notes. Lines of trans-$CH_3CH_2OCH_3$ (tEME) ground state present in the spectral scan of Orion KL from the 30 m telescope. Column 1 indicates the species, Col. 2 gives the transition, Col. 3 the predicted frequency, Col. 4 upper level energy, Col. 5 the line strength, Col. 6 observed frequency at the peak Channel of the line (relative to a v_{LSR} of +7.5 km s^{-1}), Col. 7 main beam temperature at the peak Channel of the line, and Col. 8 shows blends with other molecular species.

[1] Observed frequencies and intensities are not provided for features that appear totally blended with lines from other species.

[2] We address all features provided by our model with $T_{MB} > 0.01$ K, $T_{MB} > 0.02$ K, and $T_{MB} > 0.03$ K in the frequency ranges between 80.7–116, 122.7–150, and 150–306.7 GHz, respectively.

† Blended with previous line.

Table A.3.

Detected lines of gauche-trans-n-$CH_3CH_2CH_2OH$.

Species	Transition $J_{K_a,K_c} - J'_{K'_a,K'_c}$	Predicted frequency (MHz)	E_{upp} (K)	S_{ij}	Observed frequency (MHz)	T (K)	Blends/ Comments
G-n-propanol	$12_{7,6}$–$12_{6,6}$	124 417.241	58.0	4.25	124 417.1	0.04	30 m; U-line
G-n-propanol	$12_{7,5}$–$12_{6,6}$	124 417.256	58.0	4.89	†		
G-n-propanol	$12_{7,6}$–$12_{6,7}$	124 418.125	58.0	4.89	124 418.2†	0.06	30 m; U-line
G-n-propanol	$12_{7,5}$–$12_{6,7}$	124 418.139	58.0	4.25	†		
G-n-propanol	$15_{2,14}$–$14_{1,13}$	141 219.413	55.4	9.14	141 219.8	0.04	30 m
Gt-n-propanol	$6_{5,2}$–$5_{4,1}$	143 143.854	21.1	4.51	143 144.6	0.10	30 m; CH_3CH_2CN $v_{12} = 1$
Gt-n-propanol	$6_{5,1}$–$5_{4,1}$	143 143.873	21.1	4.65	†		
Gt-n-propanol	$6_{5,2}$–$5_{4,2}$	143 144.406	21.1	4.65	†		
Gt-n-propanol	$6_{5,1}$–$5_{4,2}$	143 144.426	21.1	4.51	†		
Gt-n-propanol	$8_{7,2}$–$7_{6,1}$	200 433.919	38.9	6.49	200 434.4	0.13	30 m
Gt-n-propanol	$8_{7,1}$–$7_{6,1}$	200 433.919	38.9	6.63	†		
Gt-n-propanol	$8_{7,2}$–$7_{6,2}$	200 433.920	38.9	6.63	†		
Gt-n-propanol	$8_{7,1}$–$7_{6,2}$	200 433.920	38.9	6.49	†		
Gt-n-propanol	$23_{11,13}$–$23_{10,13}$	200 508.301	181.2	8.64	200 508.8	0.07	30 m

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Species	Transition $J_{K_a,K_c} - J'_{K'_a,K'_c}$	Predicted frequency (MHz)	E_{upp} (K)	S_{ij}	Observed frequency (MHz)	T (K)	Blends/ Comments
Gt-n-propanol	$23_{11,12}$–$23_{10,13}$	200 508.302	181.2	10.20	†		
Gt-n-propanol	$23_{11,13}$–$23_{10,14}$	200 508.311	181.2	10.20	†		
Gt-n-propanol	$23_{11,12}$–$23_{10,14}$	200 508.312	181.2	8.64	†		
Gt-n-propanol	$9_{7,3}$–$8_{6,2}$	209 892.537	43.0	6.54	209 892.5	0.19	30 m; CH_2CHCN v_{11} = 1
Gt-n-propanol	$9_{7,2}$–$8_{6,2}$	209 892.538	43.0	6.78	†		
Gt-n-propanol	$9_{7,3}$–$8_{6,3}$	209 892.542	43.0	6.78	†		
Gt-n-propanol	$9_{7,2}$–$8_{6,3}$	209 892.542	43.0	6.54	†		
Gt-n-propanol	$24_{0,24}$–$23_{1,23}$	210 248.928	127.7	22.15	210 249.1	0.17	30 m
Gt-n-propanol	$24_{1,24}$–$23_{1,23}$	210 250.060	127.7	23.86	†		
Gt-n-propanol	$24_{0,24}$–$23_{0,23}$	210 250.810	127.7	23.86	210 252.8	0.16	30 m
Gt-n-propanol	$24_{1,24}$–$23_{0,23}$	210 251.942	127.7	22.15	†		
Gt-n-propanol	$44_{12,32}$–$44_{11,34}$	210 252.224	517.3	16.71	†		
Gt-n-propanol	$37_{12,26}$–$37_{11,26}$	215 663.302	386.2	14.57	…	…	ALMA; CH_3CH_2CN v_{13}/v_{21}
Gt-n-propanol	$37_{12,25}$–$37_{11,26}$	215 663.793	386.2	19.40	…	…	”
Gt-n-propanol	$37_{12,26}$–$37_{11,27}$	215 663.793	386.2	19.40	…	…	”
Gt-n-propanol	$37_{12,25}$–$37_{11,27}$	215 663.793	386.2	19.40	…	…	”
Gt-n-propanol	$37_{12,26}$–$37_{11,27}$	215 672.076	386.2	19.40	…	…	ALMA; CH_3COOH v_t = 1
Gt-n-propanol	$37_{12,25}$–$37_{11,27}$	215 672.568	386.2	14.57	…	…	”
Gt-n-propanol	$24_{3,21}$–$23_{4,20}$	216 493.373	143.6	9.36	…	…	ALMA; CH_3OCOH
Gt-n-propanol	$14_{5,10}$–$13_{4,9}$	217 132.672	59.3	5.22	…	…	ALMA; $CH_3O^{13}COH$ v_t = 1, CH_3OD
Gt-n-propanol	$34_{12,23}$–$34_{11,23}$	217 158.546	337.0	13.43	217 159.0	0.48	ALMA; CH_3COOCH_3
Gt-n-propanol	$34_{12,22}$–$34_{11,23}$	217 158.612	337.0	17.25	†		
Gt-n-propanol	$34_{12,23}$–$34_{11,24}$	217 159.977	337.0	17.25	†		
Gt-n-propanol	$34_{12,22}$–$34_{11,24}$	217 160.043	337.0	13.43	†		
Gt-n-propanol	$32_{12,21}$–$32_{11,21}$	217 935.916	306.4	12.61	…	…	ALMA;CH_3OCH_3, $CH_3O^{13}COH$ v_t = 1
Gt-n-propanol	$32_{12,20}$–$32_{11,21}$	217 935.931	306.4	15.85	…	…	”
Gt-n-propanol	$32_{12,21}$–$32_{11,22}$	217 936.298	306.4	15.85	…	…	”
Gt-n-propanol	$32_{12,20}$–$32_{11,22}$	217 936.314	306.4	12.61	…	…	”
Gt-n-propanol	$31_{12,20}$–$31_{11,20}$	218 268.548	291.9	12.18	218 269.0	0.84	ALMA; U-line
Gt-n-propanol	$31_{12,19}$–$31_{11,20}$	218 268.555	291.9	12.15	†		
Gt-n-propanol	$31_{12,20}$–$31_{11,21}$	218 268.739	291.9	12.15	†		
Gt-n-propanol	$31_{12,19}$–$31_{11,21}$	218 268.746	291.9	12.18	†		
Gt-n-propanol	$30_{12,19}$–$30_{11,19}$	218 567.524	277.7	11.74	…	…	ALMA; $CH_3O^{13}COH$ v_t = 1
Gt-n-propanol	$30_{12,18}$–$30_{11,19}$	218 567.527	277.7	14.45	…	…	”
Gt-n-propanol	$30_{12,19}$–$30_{11,20}$	218 567.616	277.7	14.45	…	…	”
Gt-n-propanol	$30_{12,18}$–$30_{11,20}$	218 567.619	277.7	11.74	…	…	”
Gt-n-propanol	$29_{12,18}$–$29_{11,18}$	218 835.376	264.1	11.28	218 835.5	1.05	ALMA; $CH_3^{18}OCOH$
Gt-n-propanol	$29_{12,17}$–$29_{11,18}$	218 835.377	264.1	13.76	†		
Gt-n-propanol	$29_{12,18}$–$29_{11,19}$	218 835.419	264.1	13.76	†		

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Species	Transition $J_{K_a,K_c} - J'_{K'_a,K'_c}$	Predicted frequency (MHz)	E_{upp} (K)	S_{ij}	Observed frequency (MHz)	T (K)	Blends/ Comments
Gt-n-propanol	$29_{12,17}$–$29_{11,19}$	218 835.421	264.1	11.28	†		
Gt-n-propanol	$25_{0,25}$–$24_{1,24}$	218 880.233	138.2	23.15	218 881.2	0.80	ALMA
Gt-n-propanol	$25_{1,25}$–$24_{1,24}$	218 880.912	138.2	24.86	†		
Gt-n-propanol	$25_{0,25}$–$24_{0,24}$	218 881.365	138.2	24.86	†		
Gt-n-propanol	$25_{1,25}$–$24_{0,24}$	218 882.044	138.2	23.15	†		
Gt-n-propanol	$12_{6,7}$–$11_{5,6}$	218 945.655	52.0	5.95	218 946.4	0.73	ALMA
Gt-n-propanol	$12_{6,6}$–$11_{5,6}$	218 946.539	52.0	6.77	†		
Gt-n-propanol	$12_{6,7}$–$11_{5,7}$	218 959.585	52.0	6.77	218 960.4	0.76	ALMA
Gt-n-propanol	$16_{3,14}$–$15_{2,14}$	218 960.392	65.9	5.29	†		
Gt-n-propanol	$12_{6,6}$–$11_{5,7}$	218 960.468	52.0	5.95	†		
Gt-n-propanol	$26_{4,22}$–$25_{5,21}$	219 065.066	170.6	6.54	…	…	ALMA; CH_3OCOH v_t = 1
Gt-n-propanol	$28_{12,17}$–$28_{11,17}$	219 074.469	250.9	10.82	…	…	ALMA; CH_3OCOH v_t = 1
Gt-n-propanol	$28_{12,16}$–$28_{11,17}$	219 074.470	250.9	13.07	…	…	”
Gt-n-propanol	$28_{12,17}$–$28_{11,18}$	219 074.489	250.9	13.07	…	…	”
Gt-n-propanol	$28_{12,16}$–$28_{11,18}$	219 074.490	250.9	10.82	…	…	”
Gt-n-propanol	$27_{12,16}$–$27_{11,16}$	219 287.021	238.1	10.34	…	…	ALMA; CH_3OCOH v_t = 2
Gt-n-propanol	$27_{12,15}$–$27_{11,16}$	219 287.021	238.1	12.38	…	…	”
Gt-n-propanol	$27_{12,16}$–$27_{11,17}$	219 287.030	238.1	12.38	…	…	”
Gt-n-propanol	$27_{12,15}$–$27_{11,17}$	219 287.030	238.1	10.34	…	…	”
Gt-n-propanol	$10_{7,4}$–$9_{6,3}$	219 345.954	47.6	6.62	…	…	ALMA; $CH_3O^{13}COH$
Gt-n-propanol	$10_{7,3}$–$9_{6,3}$	219 345.955	47.6	6.97	…	…	”
Gt-n-propanol	$10_{7,4}$–$9_{6,4}$	219 345.976	47.6	6.97	…	…	”
Gt-n-propanol	$10_{7,3}$–$9_{6,4}$	219 345.977	47.6	6.62	…	…	”
Gt-n-propanol	$8_{8,1}$–$7_{7,0}$	219 604.840	45.8	7.48	219 604.8	1.39	ALMA
Gt-n-propanol	$8_{8,1}$–$7_{7,0}$	219 604.840	45.8	7.52	†		
Gt-n-propanol	$8_{8,1}$–$7_{7,0}$	219 604.840	45.8	7.52	†		
Gt-n-propanol	$8_{8,1}$–$7_{7,0}$	219 604.840	45.8	7.48	†		
Gt-n-propanol	$25_{12,14}$–$25_{11,14}$	219 640.715	214.0	9.34	…	…	ALMA; CH_3OCOH v_t = 1
Gt-n-propanol	$25_{12,13}$–$25_{11,14}$	219 640.715	214.0	11.00	…	…	”
Gt-n-propanol	$25_{12,14}$–$25_{11,15}$	219 640.717	214.0	11.00	…	…	”
Gt-n-propanol	$25_{12,13}$–$25_{11,15}$	219 640.717	214.0	9.34	…	…	”
Gt-n-propanol	$22_{12,11}$–$22_{11,11}$	220 020.607	181.3	7.74	…	…	ALMA; U-line
Gt-n-propanol	$22_{12,10}$–$22_{11,11}$	220 020.607	181.3	8.91	…	…	”
Gt-n-propanol	$22_{12,11}$–$22_{11,12}$	220 020.607	181.3	8.91	…	…	”
Gt-n-propanol	$22_{12,10}$–$22_{11,12}$	220 020.607	181.3	7.74	…	…	”
Gt-n-propanol	$21_{12,10}$–$21_{11,10}$	220 113.805	171.3	7.17	220 113.2	0.81	ALMA; U-line, CH_2CHCN v_{11} = 1
Gt-n-propanol	$21_{12,9}$–$21_{11,10}$	220 113.805	171.3	7.17	†		
Gt-n-propanol	$21_{12,10}$–$21_{11,11}$	220 113.805	171.3	7.17	†		
Gt-n-propanol	$21_{12,9}$–$21_{11,11}$	220 113.805	171.3	7.17	†		
Gt-n-propanol	$18_{12,7}$–$18_{11,7}$	220 313.948	144.0	5.36	220 314.2	0.76	ALMA
Gt-n-propanol	$18_{12,6}$–$18_{11,7}$	220 313.948	144.0	6.01	†		

Species	Transition $J_{K_a,K_c} - J'_{K'_a,K'_c}$	Predicted frequency (MHz)	E_{upp} (K)	S_{ij}	Observed frequency (MHz)	T (K)	Blends/ Comments
Gt-n-propanol	$18_{12,7}$–$18_{11,8}$	220 313.948	144.0	6.01	†		
Gt-n-propanol	$18_{12,6}$–$18_{11,8}$	220 313.948	144.0	5.36	†		
Gt-n-propanol	$15_{12,4}$–$15_{11,4}$	220 422.125	120.8	3.32	220 422.3	0.65	ALMA; $^{13}CH_3OCOH$, $CH_3OC^{18}OH$
Gt-n-propanol	$15_{12,3}$–$15_{11,4}$	220 422.125	120.8	3.66	†		
Gt-n-propanol	$15_{12,4}$–$15_{11,5}$	220 422.125	120.8	3.66	†		
Gt-n-propanol	$15_{12,3}$–$15_{11,5}$	220 422.125	120.8	3.32	†		
Gt-n-propanol	$14_{12,2}$–$14_{11,3}$	220 443.126	114.0	2.82	…	…	ALMA; CH_3CH_2OH
Gt-n-propanol	$14_{12,3}$–$14_{11,3}$	220 443.126	114.0	2.57	…	…	”
Gt-n-propanol	$14_{12,2}$–$14_{11,4}$	220 443.126	114.0	2.57	…	…	”
Gt-n-propanol	$14_{12,3}$–$14_{11,4}$	220 443.126	114.0	2.82	…	…	”
Gt-n-propanol	$24_{2,22}$–$23_{3,21}$	220 450.169	139.1	14.32			ALMA; CH_3CH_2OCOH
Gt-n-propanol	$13_{12,1}$–$13_{11,3}$	220 458.292	107.6	1.77	220 458.3	0.36	ALMA
Gt-n-propanol	$13_{12,1}$–$13_{11,2}$	220 458.292	107.6	1.94	†		
Gt-n-propanol	$13_{12,2}$–$13_{11,3}$	220 458.292	107.6	1.94	†		
Gt-n-propanol	$13_{12,2}$–$13_{11,2}$	220 458.292	107.6	1.77	†		
Gt-n-propanol	$26_{0,26}$–$25_{1,25}$	227 509.942	149.1	24.15	227 510.7	1.03	ALMA
Gt-n-propanol	$26_{1,26}$–$25_{1,25}$	227 510.348	149.1	25.86	†		
Gt-n-propanol	$26_{0,26}$–$25_{0,25}$	227 510.621	149.1	25.86	†		
Gt-n-propanol	$26_{1,26}$–$25_{0,25}$	227 511.028	149.1	24.15	†		
Gt-n-propanol	$11_{7,5}$–$10_{6,4}$	228 791.566	52.6	6.71	228 791.6	1.08	ALMA
Gt-n-propanol	$11_{7,4}$–$10_{6,4}$	228 791.570	52.6	7.18	†		
Gt-n-propanol	$11_{7,5}$–$10_{6,5}$	228 791.564	52.6	7.18	†		
Gt-n-propanol	$11_{7,4}$–$10_{6,5}$	228 791.658	52.6	6.71	†		
Gt-n-propanol	$9_{8,2}$–$8_{7,1}$	229 067.766	49.9	7.49	229 066.5	2.40	ALMA; U-line
”	”	”	”	”	229 068.4	0.30	30 m
Gt-n-propanol	$9_{8,1}$–$8_{7,1}$	229 067.766	49.9	7.62	†		
Gt-n-propanol	$9_{8,2}$–$8_{7,2}$	229 067.766	49.9	7.62	†		
Gt-n-propanol	$9_{8,1}$–$8_{7,2}$	229 067.766	49.9	7.49	†		
Gt-n-propanol	$24_{3,21}$–$23_{3,20}$	229 460.087	143.6	23.32	229 462.0	0.55	ALMA
Gt-n-propanol	$25_{2,23}$–$24_{3,22}$	229 461.862	150.2	15.38	†		
Gt-n-propanol	$23_{4,20}$–$22_{3,19}$	234 033.112	133.2	8.73	234 033.2	0.74	ALMA; U-line
Gt-n-propanol	$39_{13,27}$–$39_{12,27}$	235 206.448	432.7	15.38	…	…	ALMA; CH_3OCOH $v_t = 1$
Gt-n-propanol	$39_{13,26}$–$39_{12,27}$	235 206.535	432.7	20.18	…	…	”
Gt-n-propanol	$39_{13,27}$–$39_{12,28}$	235 208.140	432.7	20.18	…	…	”
Gt-n-propanol	$39_{13,26}$–$39_{12,28}$	235 208.227	432.7	15.38	…	…	”
Gt-n-propanol	$38_{13,26}$–$38_{12,26}$	235 684.048	414.9	15.00	…	…	ALMA; DCOOH
Gt-n-propanol	$38_{13,25}$–$38_{12,26}$	235 684.093	414.9	19.46	…	…	”
Gt-n-propanol	$38_{13,26}$–$38_{12,27}$	235 684.969	414.9	19.46	…	…	”
Gt-n-propanol	$38_{13,25}$–$38_{12,27}$	235 685.014	414.9	15.00	…	…	”
Gt-n-propanol	$19_{3,16}$–$18_{2,16}$	236 101.301	92.6	8.67	…	…	ALMA; D_2CO, $CH_3{}^8OCOH$

Species	Transition $J_{K_a,K_c} - J'_{K'_a,K'_c}$	Predicted frequency (MHz)	E_{upp} (K)	S_{ij}	Observed frequency (MHz)	T (K)	Blends/ Comments
Gt-n-propanol	$37_{13,25}$–$37_{12,25}$	236 120.704	397.6	14.60	…	…	ALMA; $CH_3O^{13}COH$, CH_3OCOH $v_t = 2$
Gt-n-propanol	$37_{13,24}$–$37_{12,25}$	236 120.726	397.6	18.75	…	…	”
Gt-n-propanol	$37_{13,25}$–$37_{12,26}$	236 121.195	397.6	18.75	…	…	”
Gt-n-propanol	$37_{13,24}$–$37_{12,26}$	236 121.218	397.6	14.60	…	…	”
Gt-n-propanol	$27_{0,27}$–$26_{1,26}$	236 138.084	160.4	25.15	236 138.5	0.74	ALMA
Gt-n-propanol	$27_{1,27}$–$26_{1,26}$	236 138.327	160.4	26.86	†		
Gt-n-propanol	$27_{0,27}$–$26_{0,26}$	236 138.490	160.4	26.86	†		
Gt-n-propanol	$27_{1,27}$–$26_{0,26}$	236 138.733	160.4	25.15	†		
Gt-n-propanol	$17_{2,16}$–$16_{1,16}$	236 879.561	69.9	2.82	…	…	ALMA; CH_3OCOH
Gt-n-propanol	$35_{13,23}$–$35_{12,23}$	236 882.213	364.3	13.78	…	…	”
Gt-n-propanol	$35_{13,22}$–$35_{12,23}$	236 882.218	364.3	17.34	…	…	”
Gt-n-propanol	$35_{13,23}$–$35_{12,24}$	236 882.345	364.3	17.34	…	…	”
Gt-n-propanol	$35_{13,22}$–$35_{12,24}$	236 882.350	364.3	13.78	…	…	”
Gt-n-propanol	$34_{13,22}$–$34_{12,22}$	237 212.075	348.4	13.36	…	…	ALMA; CH_3OCOH $v_t = 2$
Gt-n-propanol	$34_{13,21}$–$34_{12,22}$	237 212.077	348.4	16.65	…	…	”
Gt-n-propanol	$34_{13,22}$–$34_{12,23}$	237 212.141	348.4	16.65	…	…	”
Gt-n-propanol	$34_{13,21}$–$34_{12,23}$	237 212.143	348.4	13.36	…	…	”
Gt-n-propanol	$14_{6,9}$–$13_{5,9}$	237 691.949	64.3	7.37	237 692.7	0.62	ALMA; $^{13}CH_3OCOH$
Gt-n-propanol	$14_{6,8}$–$13_{5,9}$	237 697.842	64.3	6.15	237 697.2	1.20	ALMA; $^{13}CH_3OCOH$ $v_t = 1$
Gt-n-propanol	$25_{3,22}$–$24_{3,21}$	237 779.216	155.0	24.29	…	…	ALMA; $^{13}CH_3OCOH$ $v_t = 1$
Gt-n-propanol	$32_{13,20}$–$32_{12,20}$	237 781.304	317.9	12.47	…	…	”
Gt-n-propanol	$32_{13,19}$–$32_{12,20}$	237 781.304	317.9	15.26	…	…	”
Gt-n-propanol	$32_{13,20}$–$32_{12,21}$	237 781.319	317.9	15.26	…	…	”
Gt-n-propanol	$32_{13,19}$–$32_{12,21}$	237 781.319	317.9	12.47	…	…	”
Gt-n-propanol	$31_{13,19}$–$31_{12,19}$	238 024.778	303.3	12.01	…	…	ALMA; CH_3OCOH $v_t = 1$
Gt-n-propanol	$31_{13,18}$–$31_{12,19}$	238 024.778	303.3	14.57	…	…	”
Gt-n-propanol	$31_{13,19}$–$31_{12,20}$	238 024.785	303.3	14.57	…	…	”
Gt-n-propanol	$31_{13,18}$–$31_{12,20}$	238 024.785	303.3	12.01	…	…	”
Gt-n-propanol	$16_{5,11}$–$15_{4,12}$	238051.137	73.5	5.21	238 051.4	0.64	ALMA
Gt-n-propanol	$37_{6,31}$–$37_{5,33}$	238 051.929	342.5	1.83	†	”	”
Gt-n-propanol	$12_{7,6}$–$11_{6,5}$	238 226.322	58.0	6.81	…	…	ALMA; CH_3OCOH $v_t = 1$
”	”	”	”	”	238 226.8	0.25	30 m; CH_3OCOH $v_t = 1$
Gt-n-propanol	$12_{7,5}$–$11_{6,5}$	238 226.337	58.0	7.42	†		
Gt-n-propanol	$12_{7,6}$–$11_{6,6}$	238226.619	58.0	7.42	†		
Gt-n-propanol	$12_{7,5}$–$11_{6,6}$	238 226.633	58.0	6.81	†		
Gt-n-propanol	$30_{13,18}$–$30_{12,18}$	238 243.369	289.2	11.53	…	…	ALMA; U-line
Gt-n-propanol	$30_{13,17}$–$30_{12,18}$	238 243.369	289.2	13.88	…	…	”
Gt-n-propanol	$30_{13,18}$–$30_{12,19}$	238 243.372	289.2	13.88	…	…	”
Gt-n-propanol	$30_{13,17}$–$30_{12,19}$	238 243.372	289.2	11.53	…	…	”
Gt-n-propanol	$26_{6,24}$–$25_{3,23}$	238 348.325	161.7	16.44	…	…	ALMA; CH_3OCOH
Gt-n-propanol	$29_{13,17}$–$29_{12,17}$	238 438.858	275.5	11.05	…	…	ALMA; CH_3OH $v_t = 1$

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Species	Transition $J_{K_a,K_c} - J'_{K'_a,K'_c}$	Predicted frequency (MHz)	E_{upp} (K)	S_{ij}	Observed frequency (MHz)	T (K)	Blends/ Comments
Gt-n-propanol	$29_{13,16}$–$29_{12,17}$	238 438.858	275.5	13.19	…	…	”
Gt-n-propanol	$29_{13,17}$–$29_{12,18}$	238 438.859	275.5	13.19	…	…	”
Gt-n-propanol	$29_{13,16}$–$29_{12,18}$	238 438.859	275.5	11.05	…	…	”
Gt-n-propanol	$10_{8,3}$–$9_{7,2}$	238 528.368	54.5	7.53	238528.6	1.01	ALMA
”	”	”	”	”	238528.8	0.18	30 m
Gt-n-propanol	$10_{8,2}$–$9_{7,2}$	238 528.368	54.5	7.76	†		
Gt-n-propanol	$10_{8,3}$–$9_{7,3}$	238 528.368	54.5	7.76	†		
Gt-n-propanol	$10_{8,2}$–$9_{7,3}$	238 528.368	54.5	7.53	†		
Gt-n-propanol	$23_{13,11}$–$23_{12,11}$	239 215.407	203.2	7.87	…	…	ALMA; $CH_3{}^{18}OCOH$
Gt-n-propanol	$23_{13,10}$–$23_{12,11}$	239 215.407	203.2	9.01	…	…	”
Gt-n-propanol	$23_{13,11}$–$23_{12,12}$	239 215.407	203.2	9.01	…	…	”
Gt-n-propanol	$23_{13,10}$–$23_{12,12}$	239 215.407	203.2	7.87	…	…	”
Gt-n-propanol	$22_{13,10}$–$22_{12,10}$	239 291.987	192.7	7.29	…	…	ALMA; CH_3OCOH $v_t = 1$
Gt-n-propanol	$22_{13,9}$–$22_{12,10}$	239 291.987	192.7	8.29	…	…	”
Gt-n-propanol	$22_{13,10}$–$22_{12,11}$	239 291.987	192.7	8.29	…	…	”
Gt-n-propanol	$22_{13,9}$–$22_{12,11}$	239 291.987	192.7	7.29	…	…	”
Gt-n-propanol	$24_{4,21}$–$23_{3,20}$	239 313.697	144.1	9.74	239 313.9	0.68	ALMA; CH_3OCOH $v_t = 2$
Gt-n-propanol	$21_{13,9}$–$21_{12,9}$	239 356.844	182.7	6.69	239 357.4	0.26	ALMA
Gt-n-propanol	$21_{13,8}$–$21_{12,9}$	239 356.844	182.7	7.56	†		
Gt-n-propanol	$21_{13,9}$–$21_{12,10}$	239 356.844	182.7	7.56	†		
Gt-n-propanol	$21_{13,8}$–$21_{12,10}$	239 356.844	182.7	6.69	†		
Gt-n-propanol	$20_{13,8}$–$20_{12,8}$	239 411.108	173.2	6.07	239 411.6	0.65	ALMA; U-line
Gt-n-propanol	$20_{13,7}$–$20_{12,8}$	239 411.108	173.2	6.83	†		
Gt-n-propanol	$20_{13,8}$–$20_{12,9}$	239 411.108	173.2	6.83	†		
Gt-n-propanol	$20_{13,7}$–$20_{12,9}$	239 411.108	173.2	6.07	†		
Gt-n-propanol	$19_{13,6}$–$19_{12,7}$	239 455.850	164.1	6.07	…	…	ALMA; U-line
Gt-n-propanol	$19_{13,7}$–$19_{12,7}$	239 455.850	164.1	5.43	…	…	”
Gt-n-propanol	$19_{13,6}$–$19_{12,8}$	239 455.850	164.1	5.43	…	…	”
Gt-n-propanol	$19_{13,7}$–$19_{12,8}$	239 455.850	164.1	6.07	…	…	”
Gt-n-propanol	$18_{13,5}$–$18_{12,6}$	239 492.090	155.5	5.30	…	…	ALMA; CH_3OCOH
Gt-n-propanol	$18_{13,6}$–$18_{12,6}$	239 492.090	155.5	4.77	…	…	”
Gt-n-propanol	$18_{13,5}$–$18_{12,7}$	239 492.090	155.5	4.77	…	…	”
Gt-n-propanol	$18_{13,6}$–$18_{12,7}$	239 492.090	155.5	5.30	…	…	”
Gt-n-propanol	$17_{13,4}$–$17_{12,5}$	239 520.792	147.3	4.51	239 520.8	0.37	ALMA
Gt-n-propanol	$17_{13,4}$–$17_{12,6}$	239 520.792	147.3	4.07	†		
Gt-n-propanol	$17_{13,5}$–$17_{12,5}$	239 520.792	147.3	4.07	†		
Gt-n-propanol	$17_{l3,5}$–$17_{l2,6}$	239 520.792	147.3	4.51	†		
Gt-n-propanol	$26_{3,24}$–$25_{2,23}$	239 523.360	161.7	16.45	239 523.8	0.44	ALMA
Gt-n-propanol	$16_{13,4}$–$16_{12,5}$	239 542.869	139.6	3.69	…	…	ALMA; CH_3OCOH
Gt-n-propanol	$16_{13,3}$–$16_{12,5}$	239 542.869	139.6	3.35	…	…	”
Gt-n-propanol	$16_{13,3}$–$16_{12,4}$	239 542.869	139.6	3.69	…	…	”

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Species	Transition $J_{K_a,K_c} - J'_{K'_a,K'_c}$	Predicted frequency (MHz)	E_{upp} (K)	S_{ij}	Observed frequency (MHz)	T (K)	Blends/ Comments
Gt-n-propanol	$16_{13,4}$–$16_{12,4}$	239 542.869	139.6	3.35	…	…	”
Gt-n-propanol	$28_{0,28}$–$27_{1,27}$	244 764.654	172.2	26.16	244 765.0	0.80	ALMA
”	”	”	”	”	244 765.0	0.08	30 m
Gt-n-propanol	$28_{1,28}$–$27_{1,27}$	244 764.799	172.2	27.86	†		
Gt-n-propanol	$28_{0,28}$–$27_{0,27}$	244 764.897	172.2	27.86	†		
Gt-n-propanol	$28_{1,28}$–$27_{0,27}$	244 765.042	172.2	26.16	†		
Gt-n-propanol	$25_{4,22}$–$24_{3,21}$	245 104.539	155.3	10.81	245 104.4	0.44	ALMA
Gt-n-propanol	$9_{9,1}$–$8_{8,0}$	248 228.722	57.7	8.48	248 228.5	0.14	30 m
Gt-n-propanol	$9_{9,0}$–$8_{8,0}$	248 228.722	57.7	8.52	†		
Gt-n-propanol	$9_{9,1}$–$8_{8,1}$	248 228.722	57.7	8.52	†		
Gt-n-propanol	$9_{9,0}$–$8_{8,1}$	248 228.722	57.7	8.48	†		
Gt-n-propanol	$14_{8,7}$–$13_{7,6}$	276 312.369	77.2	7.88	276 312.8	0.15	30 m
Gt-n-propanol	$14_{8,6}$–$13_{7,6}$	276 312.370	77.2	8.60	†		
Gt-n-propanol	$14_{8,7}$–$13_{7,7}$	276 312.417	77.2	8.60	†		
Gt-n-propanol	$14_{8,6}$–$13_{7,7}$	276 312.419	77.2	7.88	†		
Gt-n-propanol	$10_{10,1}$–$9_{9,0}$	276 842.794	71.0	9.48	276 842.8	0.10	30 m
Gt-n-propanol	$10_{10,0}$–$9_{9,0}$	276 842.794	71.0	9.52	†		
Gt-n-propanol	$10_{10,1}$–$9_{9,1}$	276 842.794	71.0	9.52	†		
Gt-n-propanol	$10_{10,0}$–$9_{9,1}$	276 842.794	71.0	9.48	†		
Gt-n-propanol	$13_{9,5}$–$12_{8,4}$	286 069.306	78.6	8.66	286 069.5	0.10	30 m
Gt-n-propanol	$13_{9,4}$–$12_{8,4}$	286 069.306	78.6	9.10	†		
Gt-n-propanol	$13_{9,5}$–$12_{8,5}$	286 069.306	78.6	9.10	†		
Gt-n-propanol	$13_{9(4}$–$12_{8(}$5	286 069.306	78.6	8.66	†		

Notes. Lines of gauche-trans-n-$CH_3CH_2CH_2OH$ (Gt–n–propanol) ground state present in the spectral scan of Orion KL from the IRAM-30 m telescope and the ALMA interferometer. Col. 1 indicates the species, Col. 2 gives the transition, Col. 3 the predicted frequency, Col. 4 upper level energy, Col. 5 the line strength, Col. 6 observed frequency at the peak channel of the line (relative to a v_{LSR} of +8.0 km s^{-1}), Col. 7 temperature at the peak channel of the line (main beam temperature for the IRAM data), and Col. 8 shows blends with other molecular species and comments.

†Blended with previous line.

References

Abdurakhmanov AA, Ragimova RA, Imanov LM. Opt. Spektrosk. 1969; 26:135. (English transl. in 1969, Opt. Spectrosc., 25, 75).

Balucani N, Ceccarelli C, Taquet V. MNRAS. 2015; 449:L16.

Brouillet N, Despois D, Baudry A, et al. A&A. 2013; 550:A46.

Brouillet N, Despois D, Lu X-H, et al. A&A. 2015 accepted.

Carroll PB, McGuire BA, Blake GA, et al. ApJ. 2015; 799:15.

Carvajal M, Margulès L, Tercero B, et al. A&A. 2009; 500:1109.

Cernicharo, J. Internal IRAM Report. IRAM; Granada: 1985.

Cernicharo, J. In: Stehl, C.; Joblin, C.; d'Hendecourt, L., editors. ECLA-2011: Proc. Europ. Conf. on Laboratory Astrophysics; Cambridge: Cambridge Univ. Press. 2012. p. 251EAS PS

Cernicharo J, Marcelino N, Roueff E, et al. ApJ. 2012; 759:L43.

Cernicharo J, Tercero B, Fuente A, et al. ApJ. 2013; 771:L10.

Coudert LH, Drouin BJ, Tercero B, et al. ApJ. 2013; 779:119.
Daly AM, Bermúdez C, López A, et al. ApJ. 2013; 768:81.
Demyk K, Mäder H, Tercero B, et al. A&A. 2007; 466:255.
Favre C, Despois D, Brouillet N, et al. A&A. 2011; 532:A32.
Feng SY, Beuther H, Henning T. A&A. 2015 accepted.
Fuchs U, Winnewisser G, Groner P, De Lucia FC, Herbst E. ApJS. 2003; 144:277.
Fuchs GW, Fuchs U, Giesen TF, Wyrowski F. A&A. 2005; 444:521.
Hayashi M, Kuwada K. J. Mol. Struct. 1975; 28:147.
Haykal I, Carvajal M, Tercero B, et al. A&A. 2014; 568:A58.
Högbom JA. A&AS. 1974; 15:417.
Kolesniková L, Tercero B, Cernicharo J, et al. ApJ. 2014; 784:L7.
López A, Tercero B, Kisiel Z, et al. A&A. 2014; 572:A44.
Maeda A, De Lucia F,C, Herbst E, et al. ApJS. 2006; 162:428.
Margulès L, Motiyenko RA, Demyk K, et al. A&A. 2009; 493:565.
Margulès L, Huet TR, Demaison J, et al. ApJ. 2010; 714:1120.
Motiyenko RA, Tercero B, Cernicharo J, Margulès L. A&A. 2012; 548:A71.
Neill JL, Steber AL, Muckle MT, et al. J. Phys. Chem. A. 2011; 115:6472. [PubMed: 21591798]
Pardo JR, Cernicharo J, Serabyn E. IEEE Trans. Antennas and Propagation. 2001; 49:12.
Peng T-C, Despois D, Brouillet N, Parise B, Baudry A. A&A. 2012; 543:A152.
Peng T-C, Despois D, Brouillet N, et al. A&A. 2013; 554:A78.
Tercero, B. Univ. Complutense de Madrid; 2012. Ph.D. Thesis
Tercero B, Cernicharo J, Pardo JR, Goicoechea JR. A&A. 2010; 517:A96.
Tercero B, Margulès L, Carvajal M, et al. A&A. 2012; 538:A119.
Tercero B, Kleiner I, Cernicharo J, et al. ApJ. 2013; 770:L13.

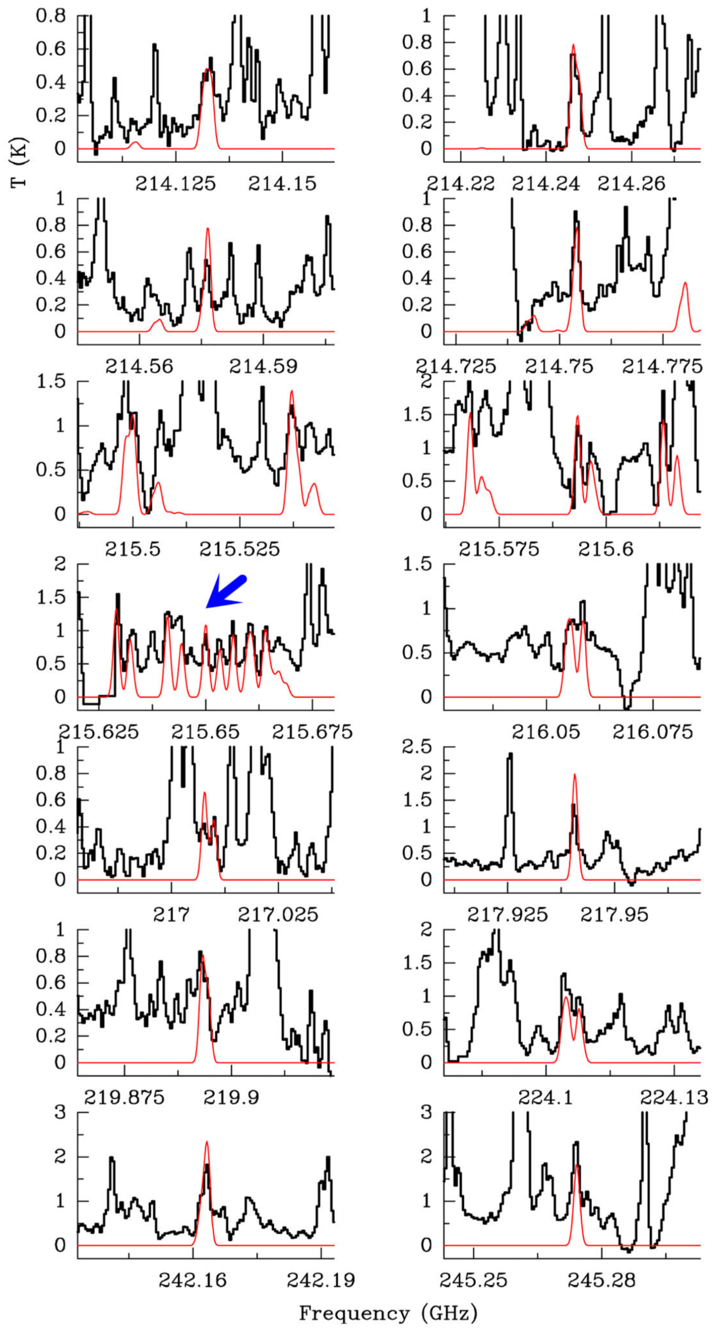

Fig. 1.

Selected lines of trans ethyl methyl ether, t-$CH_3CH_2OCH_3$, towards Orion KL detected with the ALMA interferometer in Position A (see text). A v_{LSR} of +7.5 km s^{-1} is assumed.

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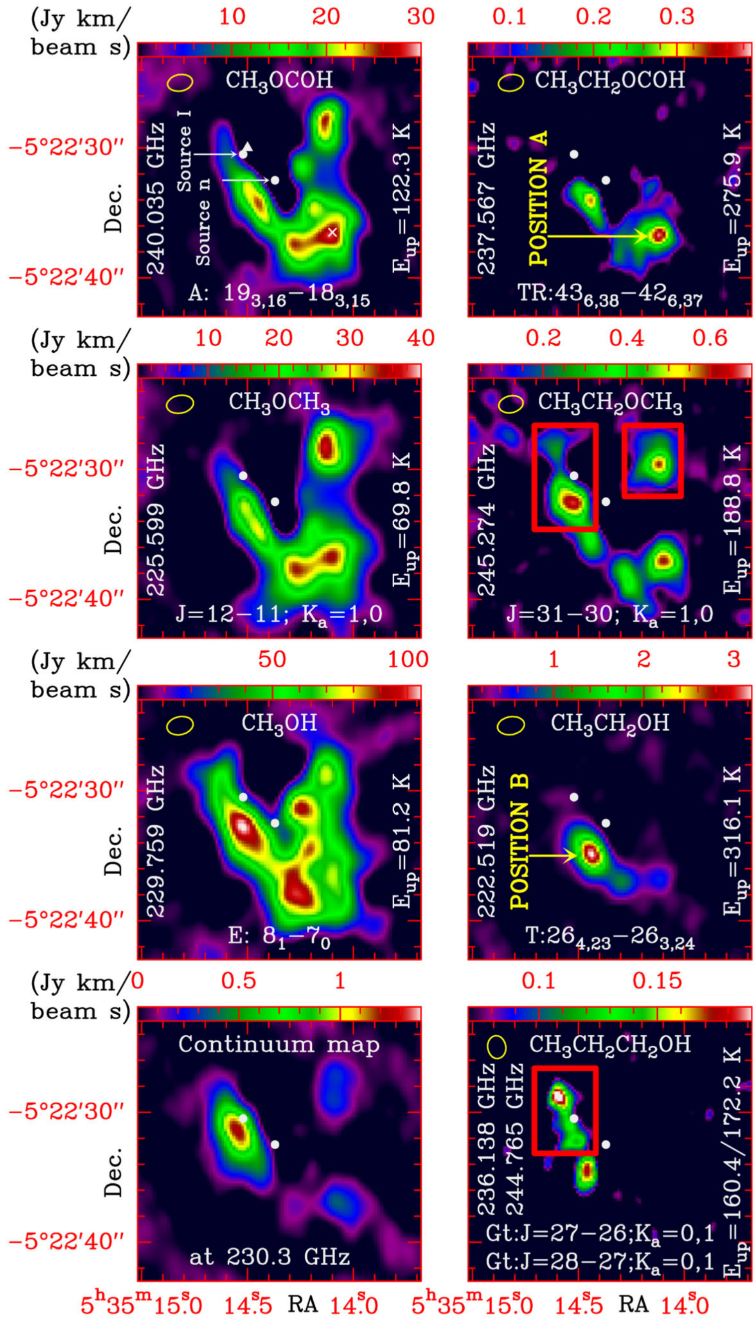

Fig. 2.

ALMA maps of organic saturated O-bearing molecules in Orion KL which have been detected containing both the methyl and the ethyl group, as well as a map of Gt-n-propanol and a continuum map at the central frequencies of the ALMA *S V* band (~230 GHz). Emission that probably arises from blended species in these maps is confined inside red rectangles. The yellow ellipse at the top left corner of the maps represents the ALMA synthetic beam. Triangle symbol: IRAM 30 m “survey position” (see Sect. 2). Cross symbol: IRAM 30 m compact ridge position (see Sect. 2). Position A: compact ridge (coordinates $\alpha_{2000.0} = 5^h35^m14^s.1$, $\delta_{2000.0} = -5°22'37''.9$). Position B: south hot core (coordinates $\alpha_{2000.0} = 5^h35^m14^s.4$, $\delta_{2000.0} = -5°22''34''.9$).

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Table 1

Column densities and ratios.

Species	$N_{g.s.}$ (×10^{15}) [cm^{-2}]	*N* Ratio
CH_3OCH_3 (DME)	600 ± 120[a,b]	
$CH_3CH_2OCH_3$ (tEME)	≤4.0 ± 0.8[a]	DME/tEME ≥ 150
$CH_3CH_2OCH_2CH_3$	≤1.0 ± 0.2[a]	DME/Tt-DEE ≥ 600
(Tt-DEE)[†]		tEME/Tt-DEE ≥ 4
CH_3OCHCH_2	≤0.5 ± 0.1[a]	DME/cis-MVE ≥ 1200
(cis-MVE)[††]		tEME/cis-MVE ≥ 9
CH_3OCOH (MF)	240 ± 50[a,b,c]	
CH_3CH_2OCOH (EF)	2.0 ± 0.4[a,d]	MF/EF ≃ 120
CH_3OH (MetOH)	2700 ± 500[b,e,f]	
CH_3CH_2OH (EtOH)	60 ± 10[b,d,e]	MetOH/EtOH ≃ 45
Gt-$CH_3CH_2CH_2OH$	1.0 ± 0.2[e]	MetOH/PropOH ≃ 2700
(PropOH)		EtOH/PropOH ≃ 60

Notes.

[†] trans-trans diethyl ether.

[††] cis methyl vinyl ether.

[a] Position A; same physical parameters of the ALMA tEME model (see Sect. 3.1).

[b] Three kinetic temperatures: 50 ± 10, 150 ± 30, and 250 ± 75 K.

[c] b type lines fitted (a type lines are optically thick); another component has been included to properly fit the observed line profiles (v_{LSR} = +9 km s^{-1}, Δv = 4 km s^{-1}, T_K = 150 ± 30 K, $N_{g.s}$ = (1.0 ± 0.2) × 10^{17}cm^{-2}).

[d] trans+gauche.

[e] Position B; assuming the same physical parameters of the ALMA Gt-n-propanol model (see Sect. 3.2).

[f] $^{12}C/^{13}C$ = 45 (Tercero et al. 2010).