

# Microwave Spectra of Molecules of Astrophysical Interest

## III. Methanol

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The available data on the microwave spectrum of methanol are critically reviewed for information applicable to radio astronomy. Molecular data such as moments and product of inertia, torsional potential constants, centrifugal distortion and torsion-rotation interaction constants, dipole moment, and structural parameters are tabulated. Observed rotational transitions are presented for the astrophysically interesting isotopic forms of methanol when available. Detailed centrifugal distortion and torsion-rotation interaction calculations have been carried out for the most abundant isotopic form of methanol. Transitions are tabulated for the frequency range from 500 MHz to 200 GHz. Measured transition error limits have been reproduced from the original literature. References are given for all data included.

Key words: Internal rotation; interstellar molecules; methanol; microwave spectra; molecular parameters; radio astronomy; rotational transitions; torsion.

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### 1. Introduction

The present tables represent the third part of a series of critical reviews [1, 2]<sup>1</sup> which are intended to update and revise the existing tabulated literature on molecules already identified in interstellar observations. The spectral information reported includes predicted as well as observed transitions between 500 MHz and 200 GHz. The reported transitions are further limited by fixing a maximum value for the total rotational and torsional energy of the lower state of the transition.

This upper limit must logically vary with the molecule being reviewed and was set at 125  $\text{cm}^{-1}$  for methanol. It is felt that this limit is generous enough to allow for the presentation of all methanol transitions which might be observed by existing telescopes. Spectral data on the less abundant isotopic forms have been included where available. Deuterated species have been purposely neglected because of the expected low cosmic abundance of the deuterium atom.

### 2. Organization of Tables

In order to reduce transcription errors, the tables of spectra have been reproduced directly from computer printout wherever possible. The open literature has been searched to October 1, 1972, for information relating to the microwave spectrum of methanol. All reports published prior to 1960 were included in Volume III of NBS Monograph 70 [3] and will not be directly referenced in the present review. Data taken from these reports are referenced MON 70.

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<sup>1</sup> Numbers in brackets indicate references in section 2.5.

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## 2.1. Molecular Parameter Table

The inertial, torsional potential, centrifugal distortion, and torsion-rotation interaction constants in table 1 were obtained from least squares analyses of the observed spectral lines with a computer program which includes these interaction terms in the computation of the rotational energies. The specific formulas used are described by Lees and Baker [4]. The molecular constants  $I_b, I_c, I_{ab}, F_v, G_v, L_v, D_{JK}$  and  $D_J$  were obtained from a least squares fit to those observed lines arising from  $\mu_a$ , the component of the dipole moment parallel to the methyl top axis, the  $a$ -axis in the internal axis system. The remaining constants were determined from a least squares fit to the hypothetical  $J = 0$  origins of  $\Delta k = 1$   $Q$  branches, which arise from the  $\mu_b$  dipole component. These were obtained by extrapolating observed series back to their origins. Because a fundamental indeterminacy exists among  $I_{a1}, I_{a2}, V_3, V_6, k_6$ , and  $k_7$ , one of them must be fixed for the nonlinear least squares fit to converge [4, 5]. The values given here correspond to  $k_7$  fixed at zero, but the large errors given for the six parameters reflect their variation with choice of the fixed parameter. The  $Q$  branch fit included a large number of infrared data, which were weighted according to the inverse square of their uncertainties.

Recently, more accurate infrared data have been obtained and a new fit was carried out [6] with the infrared data more heavily weighted relative to the microwave data. The new interaction constants give a better overall fit, but reproduce the microwave frequencies less accurately than the present constants. The available data on  $^{13}\text{CH}_3\text{OH}$  and  $\text{CH}_3^{18}\text{OH}$  were not sufficient to allow a complete least squares treatment of these species. Several of the inertial parameters for these species shown in table 1 were calculated from the structural parameters of  $^{12}\text{CH}_3^{16}\text{OH}$ . The structural parameters and electric dipole moment were taken directly from the literature cited.

## 2.2. Microwave Spectral Tables

For each spectral line the first column of table 2 contains the upper state and lower state quantum numbers in the form  $J$  and  $k$  followed by the torsional symmetry species. Transitions are ordered by symmetry with the  $A$  species listed first, followed by the  $E$  species with positive or zero  $k$ , and, finally, the  $E$  species with negative  $k$ . Lower case  $k$  is used here to denote a signed quantum number. Capital  $K$  is defined as positive or zero, with  $K = |k|$ . The  $k$   $E$  levels were previously labelled by Lees and Baker [4] as  $K E_1$  for  $k > 0$ , and  $K E_2$  for  $k < 0$ . In most instances the  $K$ -doublets are resolved for the  $A$  species so that the two components are distinguished by  $A^+$  and  $A^-$ . Transitions between the two levels of a  $K$ -doublet ( $A^+ \rightleftharpoons A^-$ ) are designated simply as  $A$ . Each symmetry type is then ordered by increasing  $J$ .

The quantum numbers are followed by the observed line frequency and, in parentheses, the experimentally estimated uncertainty in MHz. Where an experimental measurement is not available, the line frequency given is enclosed in double asterisks and is actually a calculated frequency obtained by interpolation from the calculations and observations of adjacent transitions of the same  $Q$  or  $P$  branch. The uncertainty listed is the estimated accuracy of the interpolation, which is generally substantially better than the accuracy of the computer calculated frequency, given in the third column. References to the laboratory measurements are shown in the last column of the table.

The line strengths for the rotational transitions are shown in column 4. For a transition  $J'_{k'_\sigma} \leftarrow J''_{k''_\sigma}$ , where  $\sigma$  denotes the symmetry species of the torsional state and is listed under "Species" in table 2, the line strength is defined as

$${}^x S(J'_{k'_\sigma}; J''_{k''_\sigma}) = \frac{(2J'' + 1) |\mu_{J' \leftarrow J''}|^2 \langle k'_\sigma | k''_\sigma \rangle^2}{2J''^2}$$

where the superscript  $x$  indicates the axis parallel to the dipole moment component  $\mu_x$  which produces the transition,  $|\mu_{J' \leftarrow J''}|$  indicates the dipole moment rotational matrix element connecting the upper and lower rotational levels involved in the transition, and  $\langle k'_\sigma | k''_\sigma \rangle$  indicates the torsional overlap matrix element for the two states. The line strength may be related to the Einstein coefficient  $A$  in the following manner. The probability,  $A(J'_{k'_\sigma}; J''_{k''_\sigma})$ , of a spontaneous transition per molecule in one second from the higher state,  $J'_{k'_\sigma}$ , to the lower state,  $J''_{k''_\sigma}$  is

$$A(J'_{k'_\sigma}; J''_{k''_\sigma}) = \frac{1.1639 \times 10^{-20} \nu^3 \mu_x^2}{2J'' + 1} {}^x S(J'_{k'_\sigma}; J''_{k''_\sigma}),$$

where  $\nu$  is the transition frequency in MHz and  $\mu_x$  the electric dipole component in Debye as defined above.

The total rotational and torsional energy of each level was calculated using the constants of table 1. The energies are given in columns 5 and 6 in units of  $\text{cm}^{-1}$ . Because the two torsional symmetry species do not interconvert, the zero energy for a species was chosen to be that of the lowest level of that species. The lowest energy levels, namely the  $0_0$  level for the  $A$  species and the  $1_{-1}$  level for the  $E$  species are located at  $127.817 \text{ cm}^{-1}$  and  $133.307 \text{ cm}^{-1}$ , respectively, above the bottom of the barrier to internal rotation.

As a convenience to the user, the transition frequencies from table 2 have been listed according to increasing frequency in table 3. Observed transitions for  $^{13}\text{CH}_3^{16}\text{OH}$  and  $^{12}\text{CH}_3^{18}\text{OH}$  are listed in tables 4 and 5.

## 2.3. List of Symbols and Conversion Factors

## a. Symbols

$I_{a,b,c,ab}$	Moments and product of inertia with respect to the indicated internal axis ( $\text{amu } \text{Å}^2$ ). Note that these are not principal axes.
$I_{a2}$	Moment of inertia of $\text{CH}_3$ group about its axis.
$I_{a1}$	Moment of inertia of the framework ( $I_a = I_{a1} + I_{a2}$ ).
$\Delta$	Inertial defect ( $\text{amu } \text{Å}^2$ ). $\Delta = I_c - I_{a1} - I_b$ .
$a, b, c$	Internal axes with $a$ -axis parallel to $\text{CH}_3$ symmetry axis, and $c$ -axis perpendicular to COH plane.
$V_{3,6}$	3-fold and 6-fold components of torsional barrier potential ( $\text{cm}^{-1}$ ).
$F_v, G_v, L_v$	Interaction constants for $a$ -type lines (MHz).
$D_{JK, J, K}$	Centrifugal distortion constants (MHz).
$k_1, \dots, 7$	Interaction constants for $Q$ branch origins (MHz).
$\mu_{a,b}$	Components of the dipole moment along the internal axes (Debye).
D	Abbreviation for Debye units ( $1\text{D} = 10^{-18}$ electrostatic units of charge $\times$ centimeters, or $1\text{D} = 3.33564 \times 10^{-30}$ coulomb-meter).
$r(\text{X}-\text{Y})$	Distance between centers of mass of atoms X and Y ( $\text{Å}$ ).
$\angle \text{XYZ}$	Angle formed by atoms X, Y and Z (degrees).
$\text{CH}_3$ tilt	Angle between $a$ -axis ( $\text{CH}_3$ axis) and C-O bond (degrees).
$J$	Total rotational angular momentum quantum number.
$k$	Projection of $J$ on the $a$ -axis.
$K$	Absolute value of $k$ , $K =  k $
$A \pm, E$	Torsional symmetry species. ( $\pm$ refers to $K$ -doublet).
$\sigma$	Torsional symmetry quantum number ( $\sigma = 0, +1$ for $A, E$ species).

(. . .) Parentheses in the numerical listings contain measured or estimated uncertainties. These should be interpreted as:  $1.409(0.083) = 1.409(83) = 1.409 \pm 0.083$  MHz.

## b. Conversion Factors

The following conversion factors have been used:

$$C \text{ (MHz)} = \frac{5.05375 \times 10^5}{I_c \text{ (amu } \text{Å}^2)}$$

$$1 \text{ cm}^{-1} = 29,979.25 \text{ MHz}$$

## 2.4. Acknowledgments

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## 2.5. References

- [1] Donald R. Johnson, Frank J. Lovas, and William H. Kirchhoff, *J. Phys. Chem. Ref. Data* **1**, 1011 (1972).
- [2] William H. Kirchhoff, Donald R. Johnson, and Frank J. Lovas, *J. Phys. Chem. Ref. Data* **2**, 1 (1973).
- [3] National Bureau of Standards (U.S.), Monograph 70, Vol. III (1969).
- [4] See Ref. 68A.
- [5] See Ref. 70B.
- [6] See Ref. 72B.

## 3. Methanol Spectral Tables

TABLE 1. Molecular constants for methanol

	$^{12}\text{CH}_3^{16}\text{OH}$		$^{13}\text{CH}_3^{16}\text{OH}$	$^{12}\text{CH}_3^{18}\text{OH}$
	Present work [68A]	Kwan [72B]		
Inertial constants ( $\text{amu } \text{Å}^2$ )				
$I_{a1}$	0.7536(110)	0.7530(1)	0.7496 <sup>a</sup>	0.7575 <sup>a</sup>
$I_{a2}$	3.2063(130)	3.2115(3)	3.2122 <sup>a</sup>	3.2122 <sup>a</sup>
$I_b$	20.4770(15)	...	20.9927(20) [71B]	21.3806 <sup>a</sup>
$I_c$	21.2614(17)	...	21.7774(20) [71B]	22.1730 <sup>a</sup>
$I_{ab}$	-0.065(4)	...	-0.076 <sup>a</sup>	-0.151 <sup>a</sup>
$\Delta = I_c - I_{a1} - I_b$	0.035(11)	...	0.035	0.035 <sup>a</sup>
Torsional barrier constants ( $\text{cm}^{-1}$ )				
$V_3$	373.1(3.0)	373.21(8)	376 <sup>a</sup>	376 <sup>a</sup>
$V_6$	-0.80(1.0)	-0.52(14)		
Distortion and interaction constants (MHz)				
$F_v$	-71.64(5)	...	-69.653(22) [71B]	
$G_v$	-3.501(3)	...	-3.380(3) [71B]	
$L_v$	0.068(5)	...		
$D_{JK}$	0.286(6)	...		
$D_J$	0.049(2)	...		
$D_K$	1.27(6)	1.14(9)		
$k_1$	-3.8(1.1)	-1.4(0.7)		
$k_2$	-80(3)	-55(1)		
$k_3$	-132(4)	-161(1)		
$k_4$	-249(7)	-256(2)		
$k_5$	161(23)	396(21)		
$k_6$	884(4000)	203(28)		
$k_7$	0(7000) <sup>b</sup>	0		
$^{12}\text{CH}_3^{16}\text{OH}$ Dipole moment (Debye)				
$\mu_a$	0.885 [MON70]			
$\mu_b$	1.440 [MON70]			
Structure				
$r(\text{C-H})$ Å	1.0936(32) [68A]			
$r(\text{O-H})$ Å	0.9451(34) [68A]			
$r(\text{C-O})$ Å	1.4246(24) [68A]			
$\angle \text{HCH}$	108°38'(42') [68A]			
$\angle \text{COH}$	108°32'(29') [68A]			
$\text{CH}_3$ tilt	3°16'(11') [68A]			

<sup>a</sup> Obtained by calculation from C-12 parameters with no distortion or interaction terms included.<sup>b</sup> Fixed at zero.

TABLE 2. The microwave spectrum of  $^{12}\text{CH}_3\ ^{16}\text{OH}$ 

Transition				Species	Observed frequency (estimated uncertainty)	Calculated frequency <sup>a</sup>	Line strength	Energy levels in $\text{cm}^{-1}$ <sup>b</sup>		Reference
Upper state	Lower state							Upper state	Lower state	
1	0	0	0	A+	48372.60 (.5)	48372.3	1.0000	1.614	0.0	MON70
1	1	1	1	A	834.267 (.002)	834.7	1.5000	11.733	11.705	72F
2	0	1	0	A+	96741.42 (.1)	96741.0	2.0000	4.840	1.614	68A
2	1	1	1	A+	95914.29 (.1)	95913.8	1.5000	14.904	11.705	68A
2	1	1	1	A-	97582.83 (.1)	97583.1	1.5000	14.988	11.733	68A
2	1	2	1	A	** 2502.86** (.5)	2504.1	0.8333	14.988	14.904	
2	1	3	0	A+	156602.42 (.1)	156603.2	0.9536	14.904	9.681	68A
3	0	2	0	A+	145103.23 (.1)	145102.7	3.0000	9.681	4.840	68A
3	1	2	1	A+	143865.79 (.1)	143864.9	2.6667	19.703	14.904	68A
3	1	2	1	A-	146368.30 (.1)	146369.0	2.6667	19.870	14.988	68A
3	1	3	1	A	** 5005.37 ** (.5)	5008.2	0.5833	19.870	19.703	
3	1	4	0	A+	107013.85 (.1)	107014.3	1.4305	19.703	16.133	68A
3	2	2	2	A+	145133.46 (.1)	145133.4	1.6667	35.890	31.049	68A
3	2	2	2	A-	145124.41 (.1)	145124.4	1.6667	35.890	31.049	68A
3	3	4	2	A+	** 58395.20 ** (.5)	58393.4	0.1127	44.293	42.345	
3	3	4	2	A-	** 58429.60 ** (.5)	58427.1	0.1127	44.293	42.344	
4	0	3	0	A+	193454.39 (.1)	193453.8	4.0000	16.133	9.681	68A
4	1	3	1	A+	191810.49 (.1)	191809.1	3.7500	26.101	19.703	68A
4	1	3	1	A-	195146.76 (.1)	195147.9	3.7500	26.380	19.870	68A
4	1	4	1	A	8341.64 (.1)	8346.9	0.4500	26.380	26.101	71B
4	1	5	0	A+	** 57033.30 ** (1.)	57032.5	1.9073	26.101	24.199	
4	2	3	2	A+	193511.21 (.1)	193510.8	3.0000	42.345	35.890	68A
4	2	3	2	A-	193488.03 (.1)	193488.4	3.0000	42.344	35.890	68A
4	3	3	3	A+	193471.52 (.1)	193470.4	1.7500	50.746	44.293	68A
4	3	3	3	A-	193471.52 (.1)	193470.5	1.7500	50.746	44.293	68A
4	3	5	2	A+	9978.60 (.1)	9975.8	0.2705	50.746	50.413	MON70
4	3	5	2	A-	10058.30 (.1)	10054.6	0.2705	50.746	50.411	MON70
5	1	5	1	A	12511.00 (.1)	12520.4	0.3667	34.516	34.098	MON70
5	1	6	0	A+	** 6669.30 ** (1.)	6666.3	2.3841	34.098	33.876	
5	2	6	1	A-	183853.00 (.1)	183846.1	0.7303	50.411	44.278	68A
6	1	6	1	A	17513.35 (.1)	17528.5	0.3095	44.278	43.694	MON70, 71B
6	2	5	3	A+	38452.69 (.1)	38457.1	0.4509	60.096	58.813	MON70
6	2	5	3	A-	38293.50 (.1)	38299.3	0.4509	60.096	58.813	MON70
6	2	7	1	A+	156127.70 (.1)	156140.3	0.9389	60.096	54.887	68A
6	2	7	1	A-	132621.94 (.1)	132611.6	0.9389	60.096	55.667	68A
7	0	6	1	A+	44068.80 (.1)	44074.8	2.8609	45.164	43.694	55A, 68A
7	1	7	1	A	23347.53 (.1)	23371.4	0.2679	55.667	54.887	MON70
7	2	6	3	A+	** 86902.90 ** (1.)	86909.1	0.6441	71.392	68.493	
7	2	6	3	A-	** 86615.90 ** (1.)	86624.6	0.6441	71.382	68.493	
7	2	8	1	A+	111289.62 (.1)	111309.8	1.1502	71.392	67.679	68A
7	2	8	1	A-	** 80993.10 ** (1.)	80977.8	1.1502	71.382	68.681	
8	0	7	1	A+	95169.44 (.1)	95179.7	3.3377	58.062	54.887	68A
8	1	8	1	A	** 30011.60 ** (2.)	30048.9	0.2361	68.681	67.679	
8	2	7	3	A+	135376.76 (.1)	135385.0	0.8454	84.301	79.785	68A
8	2	7	3	A-	134896.96 (.1)	134909.6	0.8454	84.285	79.785	68A
8	2	8	2	A	** 475.90 ** (.5)	471.8	0.9444	84.301	84.285	
8	2	9	1	A+	** 66948.10 ** (1.)	66979.5	1.3632	84.301	82.067	
8	2	9	1	A-	28969.90 (.1)	28946.6	1.3632	84.285	83.320	MON70, 53A
9	0	8	1	A+	146618.82 (.1)	146636.6	3.8146	72.570	67.679	68A
9	1	9	1	A	** 37502.80 ** (2.)	37561.1	0.2111	83.320	82.067	
9	2	8	3	A+	183879.96 (.1)	183890.3	1.0521	98.824	92.690	68A
9	2	8	3	A-	183123.84 (.1)	183140.8	1.0521	98.799	92.690	68A

TABLE 2. The microwave spectrum of  $^{12}\text{CH}_3^{16}\text{OH}$ —Continued

Transition				Observed frequency (estimated uncertainty)	Calculated frequency <sup>a</sup>	Line strength	Energy levels in $\text{cm}^{-1}$ <sup>b</sup>		Reference	
Upper state	Lower state		Species				Upper state	Lower state		
9	2	9	2	A	** 747.60 ** ( .5 )	741.4	0.8444	98.824	98.799	
9	2	10	1	A+	23121.20 ( .1 )	23169.6	1.5774	98.824	98.051	MON70, 62A
10	0	9	1	A+	198403.22 ( .1 )	198432.1	4.2914	88.686	82.067	68A
10	1	9	2	A-	23444.82 ( .1 )	23479.8	1.5774	99.583	98.799	MON70, 62A
10	1	10	1	A	** 45818.40 ** ( 2. )	45908.0	0.1909	99.583	98.051	
10	2	10	2	A	** 1121.40 ** ( 2. )	1112.1	0.7636	114.961	114.924	
11	1	10	2	A+	20171.07 ( .1 )	20097.8	1.7925	115.631	114.961	MON70, 68A
11	1	10	2	A-	** 76247.60 ** ( 2. )	76299.5	1.7925	117.469	114.924	
11	1	11	1	A	** 54955.60 ** ( 2. )	55089.7	0.1742	117.469	115.631	
1	0	0	0	E	48377.09 ( .5 )	48376.8	1.0000	5.246	3.632	MON70
1	1	1	0	E	165050.19 ( .1 )	165050.2	0.6482	10.751	5.246	68A
1	1	2	0	E	** 68306.30 ** ( 1. )	68305.6	0.2161	10.751	8.473	
2	0	1	0	E	96744.58 ( .1 )	96744.6	2.0000	8.473	5.246	68A
2	1	1	1	E	96755.51 ( .1 )	96755.4	1.5000	13.979	10.751	68A
2	1	2	0	E	165061.14 ( .1 )	165061.0	1.0804	13.979	8.473	68A
2	1	3	0	E	19967.30 ( .1 )	19966.7	0.4322	13.979	13.313	MON70, 59B
2	2	1	1	E	121689.85 ( .1 )	121689.4	1.3848	14.811	10.751	68A
2	2	2	1	E	24934.38 ( .1 )	24934.0	0.7693	14.811	13.979	MON70
3	0	2	0	E	145093.75 ( .1 )	145094.2	3.0000	13.313	8.473	68A
3	1	2	1	E	145131.88 ( .1 )	145132.1	2.6667	18.820	13.979	68A
3	1	2	2	E	120197.52 ( .1 )	120198.1	0.1539	18.820	14.811	68A
3	1	3	0	E	165099.31 ( .1 )	165098.9	1.5125	18.820	13.313	68A
3	2	2	1	E	170060.63 ( .1 )	170060.0	1.5386	19.651	13.979	68A
3	2	2	2	E	145126.37 ( .1 )	145126.0	1.6667	19.651	14.811	68A
3	2	3	1	E	24928.70 ( .1 )	24927.9	1.3463	19.651	18.820	MON70
4	0	3	0	E	193415.37 ( .1 )	193416.6	4.0000	19.765	13.313	68A
4	0	3	1	E	28316.03 ( .1 )	28317.8	0.6482	19.765	18.820	MON70
4	1	3	1	E	193506.60 ( .1 )	193507.7	3.7500	25.275	18.820	68A
4	1	3	2	E	**168579.20 ** ( 1. )	168579.8	0.3462	25.275	19.651	
4	1	4	0	E	165190.53 ( .1 )	165190.0	1.9447	25.275	19.765	68A
4	2	3	2	E	193511.21 ( .1 )	193511.5	3.0000	26.106	19.651	68A
4	2	4	1	E	24933.47 ( .1 )	24931.7	1.8694	26.106	25.275	MON70
4	3	3	3	E	193474.33 ( .1 )	193474.7	1.7500	43.806	37.352	68A
5	0	4	1	E	** 76509.40 ** ( 2. )	76512.8	0.8643	27.827	25.275	
5	1	5	0	E	165369.44 ( .1 )	165369.0	2.3769	33.343	27.827	68A
5	2	5	1	E	24959.08 ( .1 )	24955.6	2.3695	34.175	33.343	MON70
6	0	5	1	E	124569.97 ( .1 )	124574.5	1.0804	37.498	33.343	68A
6	1	6	0	E	165678.77 ( .1 )	165679.5	2.8090	43.025	37.498	68A
6	2	6	1	E	25018.14 ( .1 )	25012.4	2.8575	43.859	43.025	MON70
6	3	7	2	E	191733.05 ( .1 )	191721.1	0.6885	61.553	55.158	68A, 71B
7	0	6	1	E	172445.95 ( .1 )	172450.5	1.2965	48.777	43.025	68A
7	1	7	0	E	166169.21 ( .1 )	166173.5	3.2412	54.320	48.777	68A
7	2	7	1	E	25124.88 ( .1 )	25117.4	3.3383	55.158	54.320	MON70
7	3	8	2	E	143169.50 ( .1 )	143143.5	0.9037	72.847	68.072	68A, 71B
8	1	8	0	E	**166898.00 ** ( 2. )	166911.8	3.6733	67.229	61.661	
8	2	8	1	E	25294.41 ( .1 )	25288.6	3.8145	68.072	67.229	MON70
8	3	9	2	E	** 94542.00 ** ( 10. )	94486.3	1.1246	85.755	82.603	
9	1	9	0	E	**167931.00 ** ( 2. )	167964.0	4.1055	81.751	76.148	
9	2	9	1	E	25541.43 ( .1 )	25546.5	4.2876	82.603	81.751	MON70
9	3	10	2	E	45843.36 ( .1 )	45731.0	1.3495	100.275	98.750	71B
10	1	10	0	E	169335.34 ( .1 )	169408.3	4.5376	97.886	92.235	68A
10	2	10	1	E	25878.18 ( .1 )	25913.9	4.7586	98.750	97.886	MON70
11	1	11	0	E	171182.58 ( .1 )	171331.6	4.9698	115.634	109.919	68A
11	2	10	3	E	** 2932.00 ** ( 30. )	3143.4	1.5773	116.515	116.410	
11	2	11	1	E	26313.11 ( .1 )	26416.5	5.2278	116.515	115.634	MON70
0	0	1	-1	E	108893.94 ( .1 )	108894.2	0.4705	3.632	0.0	68A
1	0	1	-1	E	157270.70 ( .1 )	157271.0	0.7057	5.246	0.0	68A
1	0	2	-1	E	** 60531.70 ** ( .5 )	60532.0	0.7057	5.246	3.227	
2	0	2	-1	E	157276.04 ( .1 )	157276.7	1.1762	8.473	3.227	68A
2	0	3	-1	E	12178.60 ( .1 )	12179.5	0.9410	8.473	8.067	MON70
2	-1	1	-1	E	96739.39 ( .1 )	96739.0	1.5000	3.227	0.0	68A
3	0	3	-1	E	157272.47 ( .1 )	157274.1	1.6467	13.313	8.067	68A
3	-1	2	-1	E	145097.47 ( .1 )	145097.2	2.6667	8.067	3.227	68A

TABLE 2. The microwave spectrum of  $^{12}\text{CH}_3\ ^{16}\text{OH}$ —Continued

Transition				Observed frequency (estimated uncertainty)	Calculated frequency <sup>a</sup>	Line strength	Energy levels in $\text{cm}^{-1}$ <sup>b</sup>		Reference		
Upper state	Lower state	Species	Upper state				Lower state				
3	-2	2	-2	E	145126.37	(.1)	145126.4	1.6667	22.192	17.351	68A
4	0	4	-1	E	157246.10	(.1)	157250.0	2.1172	19.765	14.519	68A
4	-1	3	0	E	36169.24	(.1)	36167.6	1.1762	14.519	13.313	MON70
4	-1	3	-1	E	193441.62	(.1)	193441.7	3.7500	14.519	8.067	68A
4	-2	3	-2	E	193511.21	(.1)	193511.3	3.0000	28.647	22.192	68A
4	-2	5	-1	E	181771.05	(.1)	181770.4	0.5767	28.647	22.584	68A
4	-3	3	-3	E	193488.99	(.1)	193489.3	1.7500	54.230	47.776	68A
5	0	5	-1	E	157178.97	(.1)	157186.7	2.5877	27.827	22.584	68A
5	-1	4	0	E	84521.21	(.1)	84518.1	1.4115	22.584	19.765	72I
5	-2	6	-1	E	133605.50	(.1)	133602.9	0.8009	36.716	32.260	68A
6	0	6	-1	E	157048.62	(.1)	157062.0	3.0582	37.499	32.260	68A
6	-1	5	0	E	132890.79	(.1)	132885.1	1.6467	32.260	27.827	68A
6	-2	7	-1	E	** 85568.20 **	(.1)	85562.1	1.0298	46.400	43.546	
6	-4	7	-3	E	186300.95	(.1)	186297.8	0.3775	89.485	83.271	68A
7	0	7	-1	E	156828.52	(.1)	156849.4	3.5287	48.778	43.546	68A
7	-1	6	0	E	181296.03	(.1)	181286.3	1.8820	43.546	37.499	68A
7	-2	8	-1	E	37703.72	(.1)	37692.0	1.2615	57.698	56.441	MON70
7	-4	8	-3	E	137903.06	(.1)	137896.2	0.5506	100.776	96.176	68A
8	0	8	-1	E	156488.95	(.1)	156517.9	3.9992	61.662	56.441	68A
8	-4	9	-3	E	** 89505.80 **	(.1)	89494.8	0.7341	113.680	110.694	
9	0	9	-1	E	155997.52	(.1)	156032.0	4.4697	76.149	70.944	68A
9	-1	8	-2	E	9936.20	(.1)	9956.9	1.4951	70.944	70.612	MON70
10	0	10	-1	E	155320.92	(.1)	155351.9	4.9402	92.237	87.055	68A
10	-1	9	-2	E	** 57292.80 **	(.2)	57327.6	1.7300	87.055	85.142	
11	0	11	-1	E	154425.78	(.1)	154433.3	5.4106	109.921	104.770	68A
11	-1	10	-2	E	104300.46	(.1)	104356.3	1.9660	104.770	101.289	68A
12	-1	11	-2	E	150884.58	(.1)	150972.8	2.2026	124.089	119.053	68A

<sup>a</sup> The listing includes all transitions in the range 500 MHz to 200 GHz involving energy levels less than  $125\text{ cm}^{-1}$  above the lowest levels of the symmetry species.

<sup>b</sup> Heights of the ground levels above the bottom of the barrier are:  $A$  ( $J=0, K=0$ ) 127.817

$E$  ( $J=1, K=-1$ ) 133.307

<sup>c</sup> Observed frequencies enclosed in asterisks are actually hand-calculated by interpolation from the (Obs-Calc) of transitions of the same series. They represent the best calculations available.

TABLE 3. Microwave Transitions of  $^{12}\text{CH}_3\ ^{16}\text{OH}$  in order of frequency<sup>a</sup>

Frequency (MHz)	Transition			(Estimated uncertainty)	Frequency (MHz)	Transition			(Estimated uncertainty)				
	Upper state	Lower state	Species			Upper state	Lower state	Species					
** 475.90 ** <sup>b</sup>	8	2	8	2	A	(.5)	24959.08	5	2	5	1	E	(.1)
** 747.60 **	9	2	9	2	A	(.5)	25018.14	6	2	6	1	E	(.1)
834.267	1	1	1	1	A	(.002)	25124.88	7	2	7	1	E	(.1)
** 1121.40 **	10	2	10	2	A	(.2)	25294.41	8	2	8	1	E	(.1)
** 2502.86 **	2	1	2	1	A	(.5)	25541.43	9	2	9	1	E	(.1)
** 2932.00 **	11	2	10	3	E	(30.)	25878.18	10	2	10	1	E	(.1)
** 5005.37 **	3	1	3	1	A	(.5)	26313.11	11	2	11	1	E	(.1)
** 6669.30 **	5	1	6	0	A+	(.1)	28316.03	4	0	3	1	E	(.1)
8341.64	4	1	4	1	A	(.1)	28969.90	8	2	9	1	A-	(.1)
9936.20	9	-1	8	-2	E	(.1)	** 30011.60 **	8	1	8	1	A	(.2)
9978.60	4	3	5	2	A+	(.1)	36169.24	4	-1	3	0	E	(.1)
10058.30	4	3	5	2	A-	(.1)	** 37502.80 **	9	1	9	1	A	(.2)
12178.60	2	0	3	-1	E	(.1)	37703.72	7	-2	8	-1	E	(.1)
12511.00	5	1	5	1	A	(.1)	38293.50	6	2	5	3	A-	(.1)
17513.35	6	1	6	1	A	(.1)	38452.69	6	2	5	3	A+	(.1)
19967.30	2	1	3	0	E	(.1)	44068.80	7	0	6	1	A+	(.1)
20171.07	11	1	10	2	A+	(.1)	** 45818.40 **	10	1	10	1	A	(.2)
23121.20	9	2	10	1	A+	(.1)	45843.36	9	3	10	2	E	(.1)
23347.53	7	1	7	1	A	(.1)	48372.60	1	0	0	0	A+	(.5)
23444.82	10	1	9	2	A-	(.1)	48377.09	1	0	0	0	E	(.5)
24928.70	3	2	3	1	E	(.1)	** 54955.60 **	11	1	11	1	A	(.2)
24933.47	4	2	4	1	E	(.1)	** 57033.30 **	4	1	5	0	A+	(.1)
24934.38	2	2	2	1	E	(.1)	** 57292.80 **	10	-1	9	-2	E	(.2)

TABLE 3. Microwave Transitions of  $^{12}\text{CH}_3\ ^{16}\text{OH}$  in order of frequency<sup>a</sup>—Continued

Frequency (MHz)	Transition			(Estimated uncertainty)	Frequency (MHz)	Transition			(Estimated uncertainty)
	Upper state	Lower state	Species			Upper state	Lower state	Species	
** 58395.20 **	3 3	4 2	A+	(.5)	155320.92	10 0	10 -1	E	(.1)
** 58429.60 **	3 3	4 2	A-	(.5)	155997.52	9 0	9 -1	E	(.1)
** 60531.70 **	1 0	2 -1	E	(.5)	156127.70	6 2	7 1	A+	(.1)
** 66948.10 **	8 2	9 1	A+	(1.)	156488.95	8 0	8 -1	E	(.1)
** 68306.30 **	1 1	2 0	E	(1.)	156602.42	2 1	3 0	A+	(.1)
** 76247.60 **	11 1	10 2	A-	(2.)	156828.52	7 0	7 -1	E	(.1)
** 76509.40 **	5 0	4 1	E	(2.)	157048.62	6 0	6 -1	E	(.1)
** 80993.10 **	7 2	8 1	A-	(1.)	157178.97	5 0	5 -1	E	(.1)
84521.21	5 -1	4 0	E	(.1)	157246.10	4 0	4 -1	E	(.1)
** 85568.20 **	6 -2	7 -1	E	(1.)	157270.70	1 0	1 -1	E	(.1)
** 86615.90 **	7 2	6 3	A-	(1.)	157272.47	3 0	3 -1	E	(.1)
** 86902.90 **	7 2	6 3	A+	(1.)	157276.04	2 0	2 -1	E	(.1)
** 89505.80 **	8 -4	9 -3	E	(1.)	165050.19	1 1	1 0	E	(.1)
** 94542.00 **	8 3	9 2	E	(10.)	165061.14	2 1	2 0	E	(.1)
95169.44	8 0	7 1	A+	(.1)	165099.31	3 1	3 0	E	(.1)
95914.29	2 1	1 1	A+	(.1)	165190.53	4 1	4 0	E	(.1)
96739.39	2 -1	1 -1	E	(.1)	165369.44	5 1	5 0	E	(.1)
96741.42	2 0	1 0	A+	(.1)	165678.77	6 1	6 0	E	(.1)
96744.58	2 0	1 0	E	(.1)	166169.21	7 1	7 0	E	(.1)
96755.51	2 1	1 1	E	(.1)	**166898.00 **	8 1	8 0	E	(2.)
97582.83	2 1	1 1	A-	(.1)	**167931.00 **	9 1	9 0	E	(2.)
104300.46	11 -1	10 -2	E	(.1)	**168579.20 **	4 1	3 2	E	(.1)
107013.85	3 1	4 0	A+	(.1)	169335.34	10 1	10 0	E	(.1)
108893.94	0 0	1 -1	E	(.1)	170060.63	3 2	2 1	E	(.1)
111289.62	7 2	8 1	A+	(.1)	171182.58	11 1	11 0	E	(.1)
120197.52	3 1	2 2	E	(.1)	172445.95	7 0	6 1	E	(.1)
121689.85	2 2	1 1	E	(.1)	181296.03	7 -1	6 0	E	(.1)
124569.97	6 0	5 1	E	(.1)	181771.05	4 -2	5 -1	E	(.1)
132621.94	6 2	7 1	A-	(.1)	183123.84	9 2	8 3	A-	(.1)
132890.79	6 -1	5 0	E	(.1)	183853.00	5 2	6 1	A-	(.1)
133605.50	5 -2	6 -1	E	(.1)	183879.96	9 2	8 3	A+	(.1)
134896.96	8 2	7 3	A-	(.1)	186300.95	6 -4	7 -3	E	(.1)
135376.76	8 2	7 3	A+	(.1)	191733.05	6 3	7 2	E	(.1)
137903.06	7 -4	8 -3	E	(.1)	191810.49	4 1	3 1	A+	(.1)
143169.50	7 3	8 2	E	(.1)	193415.37	4 0	3 0	E	(.1)
143865.79	3 1	2 1	A+	(.1)	193441.62	4 -1	3 -1	E	(.1)
145093.75	3 0	2 0	E	(.1)	193454.39	4 0	3 0	A+	(.1)
145097.47	3 -1	2 -1	E	(.1)	193471.52	4 3	3 3	A+	(.1)
145103.23	3 0	2 0	A+	(.1)	193471.52	4 3	3 3	A-	(.1)
145124.41	3 2	2 2	A-	(.1)	193474.33	4 3	3 3	E	(.1)
145126.37	3 2	2 2	E	(.1)	193488.03	4 2	3 2	A-	(.1)
145126.37	3 -2	2 -2	E	(.1)	193488.99	4 -3	3 -3	E	(.1)
145131.88	3 1	2 1	E	(.1)	193506.60	4 1	3 1	E	(.1)
145133.46	3 2	2 2	A+	(.1)	193511.21	4 2	3 2	A+	(.1)
146368.30	3 1	2 1	A-	(.1)	193511.21	4 2	3 2	E	(.1)
146618.82	9 0	8 1	A+	(.1)	193511.21	4 -2	3 -2	E	(.1)
150884.58	12 -1	11 -2	E	(.1)	195146.76	4 1	3 1	A-	(.1)
154425.78	11 0	11 -1	E	(.1)	198403.22	10 0	9 1	A+	(.1)

<sup>a</sup> The listing includes all transitions in the range 500 MHz to 200 GHz involving energy levels less than  $125\text{ cm}^{-1}$  above the lowest levels of the symmetry species.

<sup>b</sup> Observed frequencies enclosed in asterisks are actually hand-calculated by interpolation from the (Obs-Calc) of transitions of the same series. They represent the best calculations available.

TABLE 4. Observed microwave transitions in  $^{13}\text{CH}_3^{16}\text{OH}$  (MHz)

Transition			Species	Observed frequency (estimated uncertainty)		Reference	
Upper state	Lower state						
1	0	0	0	A+	47205.20	(0.5)	MON70
2	0	1	0	A+	94407.02	(0.1)	73A
2	1	1	1	A+	93619.13	(0.1)	73A
2	1	1	1	A-	95208.67	(0.1)	73A
5	1	5	1	A	11917.74	(0.1)	71C
6	1	6	1	A	16682.72	(0.1)	71C
7	1	7	1	A	22239.91	(0.1)	72A
12	4	13	3	A+	27105.93	(0.1)	MON70
12	4	13	3	A-	26979.03	(0.1)	MON70
1	0	0	0	E	47209.63	(0.5)	MON70
2	0	1	0	E	94410.76	(0.1)	73A
2	1	1	1	E	94420.36	(0.15)	73A
2	-1	1	-1	E	94405.17	(0.15)	73A
2	1	3	0	E	23980.6	(0.5)	72A
2	2	2	1	E	27052.97	(0.1)	MON70
3	2	3	1	E	27047.19	(0.1)	MON70
4	0	3	1	F	23145.43	(0.1)	71C
4	2	4	1	E	27050.45	(0.1)	MON70
5	2	5	1	E	27072.17	(0.1)	MON70
6	2	6	1	E	27122.76	(0.1)	MON70
7	2	7	1	E	27215.60	(0.1)	MON70
8	2	8	1	E	27364.12	(0.1)	MON70
9	2	9	1	E	27581.65	(0.1)	MON70
10	2	10	1	E	27880.04	(0.1)	MON70
11	2	11	1	E	28267.71	(0.1)	MON70
12	2	12	1	E	28747.67	(0.1)	MON70
13	2	13	1	E	29315.20	(0.1)	MON70
14	2	14	1	E	29955.72	(0.1)	MON70
15	2	15	1	E	30643.69	(0.1)	MON70

TABLE 5. Observed microwave transitions in  $^{12}\text{CH}_3^{18}\text{OH}$  (MHz)

Transition			Species	Observed frequency (estimated uncertainty)		Reference	
Upper state	Lower state						
2	2	2	1	E	33918.97	(0.1)	MON70
3	2	3	1	E	33925.49	(0.1)	MON70
4	2	4	1	E	33943.63	(0.1)	MON70
5	2	5	1	E	33981.35	(0.1)	MON70
6	2	6	1	E	34048.42	(0.1)	MON70
7	2	7	1	E	34155.63	(0.1)	MON70
8	2	8	1	E	34314.64	(0.1)	MON70
9	2	9	1	E	34536.74	(0.1)	MON70
10	2	10	1	E	34831.64	(0.1)	MON70
11	2	11	1	E	35206.11	(0.1)	MON70
12	2	12	1	E	35661.78	(0.1)	MON70
13	2	13	1	E	36193.55	(0.1)	MON70
14	2	14	1	E	36787.33	(0.1)	MON70
15	2	15	1	E	37418.97	(0.1)	MON70

3.1.  $\text{CH}_3\text{OH}$  References

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