

Microwave Spectra of Molecules of Astrophysical Interest

XV. Propyne

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The microwave spectrum of propyne is critically reviewed for information applicable to radio-astronomy. Molecular data such as the derived rotational constants, centrifugal distortion parameters, hyperfine coupling constants, electric dipole moment, and molecular structure are tabulated. The observed rotational transitions are presented for the astronomically interesting isotopic forms and the lowest lying vibrational state of propyne. Calculated rotational transitions are presented for the ground vibrational state of $^{12}\text{CH}_3\text{C} \equiv ^{12}\text{CH}$, $^{13}\text{CH}_3\text{C} \equiv ^{12}\text{CH}$, $^{12}\text{CH}_3\text{C} \equiv ^{12}\text{CH}$ and $^{12}\text{CH}_3\text{C} \equiv ^{13}\text{CH}$, and for the vibrationally excited state ν_{10} of $^{12}\text{CH}_3\text{C} \equiv ^{12}\text{CH}$.

Key words: Interstellar molecules; line strengths; microwave spectra; molecular constants; propyne; radio astronomy; rotational transitions.

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1. Introduction

The present work is part of a series of critical reviews which are intended to update, revise, and augment the existing literature on molecules which have been identified in interstellar molecular clouds. In order to provide complete coverage of the spectral regions where present and anticipated radio telescope receivers operate, all measured and predicted rotational transitions are included up to 300 GHz.

2. Organization of the Spectral Tables

The molecular constants for the ground vibrational state of the isotopic forms of propyne considered in this work are given in table 1; those for the ν_{10} excited state of the most

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abundant isotopic species are given in table 6. The microwave spectral transitions of each of the propyne species are listed separately in table 2 through table 5; those for the ν_{10} state are listed in table 7. Table 8 contains a list of the strongest calculated transitions reported here, ordered by increasing frequency as an aid to the user.

The open literature relating to laboratory and astronomical studies of $\text{CH}_3\text{C} \equiv \text{CH}$ has been searched through May 1978. All pertinent references are given in section 3.

2.1. Molecular Parameter Tables

The rotational and centrifugal distortion constants for $^{12}\text{CH}_3\text{C} \equiv ^{12}\text{CH}$, $^{13}\text{CH}_3\text{C} \equiv ^{12}\text{CH}$, $^{12}\text{CH}_3\text{C} \equiv ^{12}\text{CH}$ and $^{12}\text{CH}_3\text{C} \equiv ^{13}\text{CH}$ are given in table 1. Other pertinent molecular parameters are also found in table 1. The rotational, centrifugal distortion and vibration rotation interaction con-

stants for the ν_{10} degenerate vibrational excited state of $^{12}\text{CH}_3\ ^{12}\text{C} \equiv ^{12}\text{CH}$ are given in table 6.

A full description of the theory of rotational spectra is given in a number of texts, but the books by Townes and Schawlow [1]¹, Gordy and Cook [2], Amat, Nielsen, and Tarrago [3], and Kroto [4] are particularly thorough and the notation used here is generally consistent with these texts.

The spectroscopic constants of the ground states of the various isotopic species were derived using the following expression for the frequency of a rotational $J+1, K \leftarrow J, K$ transition,

$$\begin{aligned} \nu = & 2B_0(J+1) - 4D_J(J+1)^3 - 2D_{JK}(J+1)K^2 \\ & + H_{JJ}(J+1)^3[(J+2)^3 - J^3] + 4H_{JK}(J+1)K^2 \\ & + 2H_{KK}(J+1)K^4 \end{aligned}$$

The lowest fundamental vibration of the propyne molecule is the C—C≡C bending mode (ν_{10} : 328 cm⁻¹ [5]). This vibration is doubly degenerate having E vibrational symmetry. This introduces an internal vibrational angular momentum characterized by the l quantum number, which removes the K degeneracy. For a $v_E=1$ state, $|l|=1$, higher order calculations of the energy introduce “ l type doubling” effects which involve splittings of all the K lines according to the positive or negative value of the Kl product, and a further splitting of those states for which $K=l=\pm 1$.

For molecules with a threefold symmetry axis, the rotational frequency of a $J+1, K, l \leftarrow J, K, l$ transition is given by the following expression:

$$\begin{aligned} \nu = & 2B_v^*(J+1) - 4D_J(J+1)^3 - 2D_{JK}(J+1)(Kl-1)^2 \\ & + 2\rho^*(J+1)(Kl-1) \\ & \pm 4q(J+1) \text{ if } Kl=+1 \\ & \frac{-4q^2}{(Kl-1)(B-A+A\zeta^2)} \text{ if } Kl \neq 1 \end{aligned}$$

The convention of Amat, Nielsen and Tarrago [3] has been adopted, where

$$\begin{aligned} B^* = & B_v - D_{JK} + \eta_J + 12 \frac{q_{12}}{B-A-2A\zeta^2} \\ \rho^* = & \eta_J - 2D_{JK} + \frac{2q^2}{B-A+A\zeta^2} + \frac{8(q_{12})^2}{B-A-2A\zeta^2} \end{aligned}$$

as proposed by Grenier-Besson [6]. These authors use for the l -type doubling constant, q , a definition different from that given in standard text books [1] [2], the q constant given by Amat et al. [3] being four times smaller.

For each spectrum, a weighted least-squares fitting of all observed transitions was carried out. Each datum was assigned a weight equal to the reciprocal of the square of its estimated uncertainty.

2.2. Microwave Spectral Tables

The results of the statistical analysis of the rotational spectrum of the various isotopic species of propyne and the lowest lying vibrational state of the most abundant isotopic species are given in tables 2, 3, 4, 5, and 7. The frequencies included in these tables include all transitions with sufficient intensity over the range 16 to 300 GHz. The first columns give the upper and lower state rotational quantum numbers of the transition in question. If vibrational angular momentum exists, the l quantum numbers are also included. The observed line frequency follows next. The calculated frequencies and statistical uncertainty (one standard deviation) follow in the next column.

Values of the line strength of each transition are also included in the table. They are calculated using the following expression:

$$S(J', J'') = \frac{J'^2 - K^2}{J'}$$

For the ground state transitions, the approximate energy of the lowest level has been derived from the constants of table 1. For these computations, the A axial rotational constant, which could not be obtained experimentally, has been calculated from the structure [73A]. For the same reason, the D_K centrifugal distortion constant has been obtained from the force field [76A]. The sextic centrifugal distortion constants have been neglected. For the excited state, the energy levels could not be given, because the ω_u anharmonic constant, which is of the same order of magnitude as the A constant, is not known.

For the convenience of the user, the frequencies of the strongest transitions calculated in this work are arranged in numerical order in table 8; this tabulation has been arbitrarily limited to the $K \leq 3$ transitions, which are the strongest for each isotopic species.

2.3. List of Symbols

A_v, B_v	Rotational constants for the ground ($v=0$) or excited state ($v \neq 0$).
D_J, D_{JK}, D_K	Quartic centrifugal distortion constants.
H_{JJ}, H_{JK}, H_{KK}	Sextic centrifugal distortion constants.
q	l -type doubling constant. Coefficient of the $\langle K, l H K \pm 1, l \pm 2 \rangle$ element in the energy matrix.
q_{12}	Coefficient of the $\langle K, l H K \pm 1, l \mp 2 \rangle$ element in the energy matrix.
η_J	Coefficient of the $J(J+1) K$ diagonal contribution in the energy matrix.
ζ^2	Coriolis coupling constant.
ω_u	Anharmonic vibrational constant (l^2 term).
J	Total rotational quantum number.
K	Projection of J on the symmetry axis.
σ_l	Quantum number for vibrational angular momentum.

¹Figures in brackets indicate literature references.

ν_t	Quantum number for the t^{th} vibrational state.	$\alpha^{\circ}(XYZ)$	Angle formed by atoms X, Y, and Z (degrees).
μ_0	Electric dipole moment in the ground vibrational state.	(. . .)	Parentheses in the numerical listings contain measured uncertainties or standard deviations for calculated quantities.
g_{\perp}, g_{\parallel}	Components of the molecular G tensor which are respectively perpendicular and parallel to the symmetry axis.		
X_{\perp}, X_{\parallel}	Components of the magnetic susceptibility tensor which are respectively perpendicular and parallel to the symmetry axis.		
Θ_{\parallel}	Component of the molecular quadrupole tensor which is parallel to the symmetry axis.		
$r^{\circ}(X-Y)$	Distance between centers of mass of atoms X and Y (\AA).		

2.4. References

- [1] C. H. Townes and A. L. Schawlow, *Microwave Spectroscopy*, McGraw-Hill, New York, 1955.
- [2] W. Gordy and R. L. Cook, *Microwave Molecular Spectra*, John Wiley and Sons, New York, 1970.
- [3] G. Amat, H. H. Nielsen, and G. Tarrago, *Rotation-vibration of Polyatomic Molecules*, Dekker, New York, 1971.
- [4] H. W. Kroto, *Molecular Rotation Spectra*, John Wiley and Sons, New York, 1975.
- [5] D. R. Boyd and H. W. Thompson, *Trans. Faraday Soc.* **48**, 493 (1952).
- [6] M. L. Grenier-Besson and G. Amat. *J. Mol. Spectrosc.* **8**, 22, (1962).

3. Propyne Spectral Tables

TABLE 1. Molecular constants for propyne (ground state)

	${}^{12}\text{CH}_3 {}^{12}\text{C} \equiv {}^{12}\text{CH}$	${}^{13}\text{CH}_3 {}^{12}\text{C} \equiv {}^{12}\text{CH}$	${}^{12}\text{CH}_3 {}^{13}\text{C} \equiv {}^{12}\text{CH}$	${}^{12}\text{CH}_3 {}^{12}\text{C} \equiv {}^{13}\text{CH}$
$B_0(\text{MHz})$	8 545.877 12 (6)	8 313.246 89 (215)	8 542.332 06 (168)	8 290.249 81 (160)
$D_J(\text{kHz})$	2.942 3 (7)	2.796 (23)	2.936 (17)	2.801 (16)
$D_K(\text{kHz})$	163.423 (10)	155.201 (61)	162.857 (59)	155.533 (57)
$D_K(\text{kHz})^a$	2 983 [76A]	2 991 [76A]	2 984 [76A]	2 991 [76A]
$H_{JJ}(\text{Hz})$	0.0097 (20)	-0.044 (62)	-0.048 (50)	0.117 (45)
$H_{JK}(\text{Hz})$	0.935 (68)	0.84 (20)	1.24 (21)	0.78 (18)
$H_{KK}(\text{Hz})$	5.23 (14)	5.09 (67)	4.80 (38)	5.56 (57)

Dipole moment ^b for ${}^{12}\text{CH}_3 {}^{12}\text{C} \equiv {}^{12}\text{CH}$

$$\mu_0(\text{Debyes}) = 0.7804 [66A]$$

Magnetic constants for ${}^{12}\text{CH}_3 {}^{12}\text{C} \equiv {}^{12}\text{CH}$

$$g_{\perp} = 0.00350 (15) [69B]$$

$$g_{\parallel} = 0.295 [75A]$$

$$X_{\perp} - X_{\parallel} (\text{erg}/\text{G}^2 \text{ mol}) = 7.74 (14) \times 10^{-6} [69B]$$

$$\theta_{\parallel} (\text{esu cm}^3) = 4.82 (23) \times 10^{-26}$$

Structure [73A]

$$r^{\circ} (\text{C}-\text{H}) = 1.096 (2) \text{ \AA}; r^{\circ} (\text{C}-\text{C}) = 1.4596 (10) \text{ \AA}; r^{\circ} (\text{C} \equiv \text{C}) = 1.2073 (10) \text{ \AA}; r^{\circ} (= \text{C}-\text{H}) = 1.060 (2) \text{ \AA}; \\ a^{\circ} (\text{HCH}) = 108^{\circ} 17' (15)$$

^a Calculated from the force field.

^b Polarity determined to be ${}^+ \text{CH}_3 \text{C} \equiv \text{CH}^-$ [69B].

TABLE 2 Microwave Spectrum of $^{12}\text{CH}_3\ ^{12}\text{C} \equiv ^{12}\text{CH}$ in the Ground Vibrational State.

Transition $J'K' \leftarrow J''K''$	Obs. Freq. in MHz (Est. Unc.)	Calc. Freq. in MHz (Est. Unc.)	Line Strength	Approximate Energy in cm^{-1} Lower State	Ref.
10+00		17 091.742 5(2)	1.000	0.000	
20+10	34 183.420 (50)	34 183.414 3(5)	2.000	0.570	69A
21+11	34 182.755 (50)	34 182.760 7(4)	1.500	5.422	69A
30+20	51 274.75 (10)	51 274.945 0(6)	3.000	1.710	50A
31+21	51 273.76 (10)	51 273.964 6(6)	2.667	6.562	50A
32+22	51 270.86 (10)	51 271.023 7(6)	1.667	21.116	50A
40+30	68 366.230 (30)	68 366.263 8(7)	4.000	3.421	69A
41+31	68 364.955 6(10)	68 364.956 7(7)	3.750	8.272	78A
42+32	68 361.035 1(10)	68 361.035 9(7)	3.000	22.826	78A
43+33	68 354.502 (5)	68 354.502 9(13)	1.750	47.078	78A
50+40	85 457.272 (60)	85 457.300 2(7)	5.000	5.701	69A
51+41	85 455.622 (60)	85 455.666 5(6)	4.800	10.553	69A
52+42	85 450.730 (60)	85 450.766 0(7)	4.200	25.106	69A
53+43	85 442.528 (60)	85 442.600 6(14)	3.200	49.358	69A
54+44	85 431.224 (60)	85 431.173 4(27)	1.800	83.303	69A
60+50	102 547.984 2(10)	102 547.983 7(6)	6.000	8.552	78A
61+51	102 546.024 1(10)	102 546.023 5(5)	5.833	13.403	78A
62+52	102 540.144 7(20)	102 540.143 7(7)	5.333	27.957	78A
63+53	102 530.348 7(30)	102 530.346 4(14)	4.500	52.209	78A
64+54	102 516.573 (90)	102 516.635 5(28)	3.333	86.153	69A
65+55	102 499.110 (90)	102 499.016 2(49)	1.833	129.781	69A
70+60	119 638.243 6(10)	119 638.243 8(5)	7.000	11.972	78A
71+61	119 635.958 3(15)	119 635.957 3(4)	6.857	16.824	78A
72+62	119 629.100 5(20)	119 629.098 4(6)	6.429	31.377	78A
73+63	119 617.671 (5)	119 617.670 0(14)	5.714	55.629	78A
74+64	119 601.726 (60)	119 601.676 3(27)	4.714	89.572	69A
75+65	119 581.168 (60)	119 581.123 6(48)	3.429	133.200	69A
76+66	119 556.066 (60)	119 556.019 6(79)	1.857	186.501	69A
80+70	136 728.009 8(5)	136 728.010 0(5)	8.000	15.963	78A
81+71	136 725.396 6(10)	136 725.397 2(4)	7.875	20.814	78A
82+72	136 717.559 6(15)	136 717.559 9(6)	7.500	35.367	78A
83+73	136 704.501 6(20)	136 704.501 1(13)	6.875	59.619	78A
84+74	136 686.19 (30)	136 686.225 8(25)	6.000	93.562	57A
85+75	136 662.74 (30)	136 662.740 9(43)	4.875	137.189	57A
86+76	136 634.03 (30)	136 634.055 6(72)	3.500	190.489	57A
87+77	136 600.15 (30)	136 600.180 9(118)	1.875	253.449	57A
90+80	153 817.211 7(10)	153 817.211 9(6)	9.000	20.524	78A
91+81	153 814.273 2(10)	153 814.273 1(6)	8.889	25.375	78A
92+82	153 805.457 5(15)	153 805.457 8(8)	8.556	39.928	78A
93+83	153 790.768 8(15)	153 790.769 5(15)	8.000	64.179	78A
94+84	153 770.224 (30)	153 770.213 7(25)	7.222	98.121	78A
95+85	153 743.800 (30)	153 743.798 5(40)	6.222	141.747	78A
96+86	153 711.520 (30)	153 711.533 8(63)	5.000	195.046	78A
97+87	153 673.424 (30)	153 673.432 2(102)	3.556	258.005	78A
98+88	153 629.472 (50)	153 629.508 3(167)	1.889	330.608	78A
10,0+90	170 905.66 (35)	170 905.779 0(9)	10.000	25.655	57A
10,1+91	170 902.37 (35)	170 902.514 4(9)	9.900	30.506	57A
10,2+92	170 892.59 (35)	170 892.721 8(11)	9.600	45.058	57A
10,3+93	170 876.27 (35)	170 876.405 0(20)	9.100	69.308	57A
10,4+94	170 853.50 (35)	170 853.570 3(32)	8.400	103.250	57A
10,5+95	170 824.13 (35)	170 824.226 3(44)	7.500	146.876	57A
10,6+96	170 788.29 (35)	170 788.384 5(59)	6.400	200.174	57A
10,7+97	170 746.05 (35)	170 746.058 7(86)	5.100	263.131	57A
10,8+98		170 697.265 0(138)	3.600	335.732	
10,9+99		170 642.022 4(230)	1.900	417.960	
11,0+10,0	187 993.69 (40)	187 993.641 2(13)	11.000	31.355	57A
11,1+10,1	187 990.02 (40)	187 990.051 0(12)	10.909	36.206	57A
11,2+10,2	187 979.34 (40)	187 979.281 8(16)	10.636	50.759	57A
11,3+10,3	187 961.41 (40)	187 961.337 6(29)	10.182	75.008	57A
11,4+10,4	187 936.34 (40)	187 936.225 4(47)	9.545	108.949	57A
11,5+10,5	187 903.96 (40)	187 903.954 9(64)	8.727	152.574	57A
11,6+10,6	187 864.42 (40)	187 864.538 4(78)	7.727	205.871	57A
11,7+10,7	187 817.95 (40)	187 817.991 1(92)	6.545	268.827	57A
11,8+10,8	187 763.96 (40)	187 764.331 1(119)	5.182	341.426	57A
11,9+10,9		187 703.578 9(187)	3.636	423.652	
11,10+10,10		187 635.758 0(314)	1.909	515.483	
12,0+11,0	205 080.660 (50)	205 080.728 2(16)	12.000	37.626	78A
12,1+11,1	205 076.775 (50)	205 076.812 7(16)	11.917	42.477	78A
12,2+11,2	205 065.015 (50)	205 065.067 5(22)	11.667	57.029	78A
12,3+11,3	205 045.401 (50)	205 045.497 2(43)	11.250	81.278	78A
12,4+11,4	205 018.080 (50)	205 018.109 3(71)	10.667	115.218	78A
12,5+11,5	204 982.869 (50)	204 982.914 3(100)	9.917	158.842	78A
12,6+11,6	204 939.908 (50)	204 939.925 9(124)	9.000	212.137	78A
12,7+11,7	204 889.088 (40)	204 889.160 5(140)	7.917	275.091	78A
12,8+11,8		204 830.637 7(151)	6.667	347.689	
12,9+11,9	204 764.348 (50)	204 764.380 2(179)	5.250	429.913	78A

TABLE 2 Microwave Spectrum of $^{12}\text{CH}_3\ ^{12}\text{C} \equiv ^{12}\text{CH}$ in the Ground Vibrational State (continued).

Transition $J'K' \leftarrow J''K''$	Obs. Freq. in MHz (Est. Unc.)	Calc. Freq. in MHz (Est. Unc.)	Line Strength	Approximate Energy in cm^{-1} Lower State	Ref.
12,10+11,10	204 690.354(50)	204 690.413 4 (263)	3.667	521.742	78A
12,11+11,11	204 608.766 0 (432)	1.917	623.153		
13,0+12,0	222 166.970(5)	222 166.969 8 (23)	13.000	44.467	78A
13,1+12,1	222 162.46(45)	222 162.729 2 (22)	12.923	49.318	57A
13,2+12,2	222 149.80(45)	222 150.008 9 (33)	12.692	63.869	57A
13,3+12,3	222 128.808(50)	222 128.813 8 (63)	12.308	88.118	78A
13,4+12,4	222 099.05(45)	222 099.152 1 (104)	11.769	122.057	57A
13,5+12,5	222 060.95(45)	222 061.035 2 (148)	11.077	165.679	57A
13,6+12,6	222 014.448(50)	222 014.477 7 (190)	10.231	218.973	78A
13,7+12,7	221 959.38(45)	221 959.497 7 (223)	9.231	281.926	57A
13,8+12,8		221 896.116 3 (243)	8.077	354.522	
13,9+12,9	221 824.368(50)	221 824.357 9 (254)	6.769	436.743	78A
13,10+12,10		221 744.250 3 (283)	5.308	528.569	
13,11+12,11		221 655.824 4 (283)	3.692	629.978	
13,12+12,12		221 559.114 6 (603)	1.923	740.944	
14,0+13,0	239 252.296 3 (30)	239 252.296 0 (35)	14.000	51.878	78A
14,1+13,1	239 247.727 2 (70)	239 247.730 6 (35)	13.929	56.728	78A
14,2+13,2	239 234.011(20)	239 234.036 0 (50)	13.714	71.279	78A
14,3+13,3	239 211.216(20)	239 211.217 6 (89)	13.357	95.527	78A
14,4+13,4	239 179.248(30)	239 179.284 2 (146)	12.857	129.465	78A
14,5+13,5	239 138.04(50)	239 138.247 9 (211)	12.214	173.086	57A
14,6+13,6	239 088.144(30)	239 088.124 7 (277)	11.429	226.379	78A
14,7+13,7		239 028.933 8 (335)	10.500	289.330	
14,8+13,8	238 960.752(60)	238 960.698 0 (379)	9.429	361.923	78A
14,9+13,9	238 883.496(60)	238 883.443 8 (404)	8.214	444.142	78A
14,10+13,10		238 797.200 9 (418)	6.857	535.966	
14,11+13,11		238 702.002 8 (453)	5.357	637.372	
14,12+13,12	238 597.896(60)	238 597.886 2 (578)	3.714	748.334	78A
14,13+13,13	238 484.892(90)	238 484.891 7 (850)	1.929	868.827	78A
15,0+14,0		256 336.636 8 (57)	15.000	59.858	
15,1+14,1		256 331.746 9 (58)	14.933	67.709	
15,2+14,2		256 317.079 0 (76)	14.733	79.259	
15,3+14,3		256 292.638 9 (125)	14.400	103.506	
15,4+14,4		256 258.435 8 (200)	13.933	137.444	
15,5+14,5		256 214.483 0 (289)	13.333	181.063	
15,6+14,6		256 160.797 5 (383)	12.600	234.354	
15,7+14,7		256 097.399 8 (474)	11.733	297.303	
15,8+14,8		256 024.314 5 (553)	10.733	369.894	
15,9+14,9		255 941.569 7 (609)	9.600	452.111	
15,10+14,10		255 849.197 6 (642)	8.333	543.931	
15,11+14,11		255 547.233 7 (662)	6.933	645.334	
15,12+14,12		255 635.717 7 (710)	5.400	756.293	
15,13+14,13		255 514.692 7 (865)	3.733	876.781	
15,14+14,14		255 384.205 9 (1201)	1.933	1 067.692	
16,0+15,0	273 419.922 3 (91)	16.000	68.409		
16,1+15,1	273 414.708 3 (93)	15.937	73.259		
16,2+15,2	273 399.068 1 (114)	15.750	87.809		
16,3+15,3	273 373.007 9 (174)	15.437	112.055		
16,4+15,4	273 336.537 6 (267)	15.000	145.991		
16,5+15,5	273 289.671 3 (384)	14.437	189.609		
16,6+15,6	273 232.427 1 (512)	13.750	242.898		
16,7+15,7	273 164.827 0 (643)	12.937	305.845		
16,8+15,8	273 086.897 2 (763)	12.000	378.434		
16,9+15,9	272 998.667 6 (864)	10.937	460.648		
16,10+15,10	272 900.172 6 (937)	9.750	552.465		
16,11+15,11	272 791.450 1 (981)	8.437	653.864		
16,12+15,12	272 672.542 3 (1011)	7.000	764.820		
16,13+15,13	272 543.495 4 (1079)	5.437	885.304		
16,14+15,14	272 404.359 5 (1273)	3.750	1 015.288		
16,15+15,15	272 255.188 9 (1685)	1.937	1 154.738		
17,0+16,0	290 502.082 7 (140)	17.000	77.529		
17,1+16,1	290 496.544 9 (143)	16.941	82.379		
17,2+16,2	290 479.933 5 (168)	16.765	96.929		
17,3+16,3	290 452.255 0 (237)	16.471	121.174		
17,4+16,4	290 413.520 0 (352)	16.059	155.109		
17,5+16,5	290 363.743 5 (499)	15.529	198.725		
17,6+16,6	290 302.944 6 (666)	14.882	252.012		
17,7+16,7	290 231.146 8 (842)	14.118	314.957		
17,8+16,8	290 148.377 8 (1014)	13.235	387.543		
17,9+16,9	290 054.669 6 (1168)	12.235	469.754		
17,10+16,10	289 950.058 4 (1295)	11.118	561.568		
17,11+16,11	289 834.584 8 (1387)	9.882	662.964		
17,12+16,12	289 708.293 5 (1445)	8.529	773.915		
17,13+16,13	289 571.233 6 (1492)	7.059	894.395		
17,14+16,14	289 423.458 4 (1587)	5.471	1 024.374		
17,15+16,15	289 265.025 4 (1833)	3.765	1 163.819		
17,16+16,16	289 095.996 5 (2335)	1.941	1 312.696		

TABLE 3 Microwave Spectrum of $^{13}\text{CH}_3$ - $^{12}\text{C} \equiv$ ^{12}CH in the Ground Vibrational State

Transition $J'K' \leftarrow J''K''$	Obs. Freq. in MHz (Est. Unc.)	Calc. Freq. in MHz (Est. Unc.)	Line Strength	Approximate Energy in cm^{-1} Lower State	Ref.
1,0 0,0		16 626.483 (8)	1.000	0.00	
2,0 1,0	33 252.88 (3)	33 252.898 (16)	2.000	0.55	78A,50A
2,1 1,1	33 252.22 (3)	33 252.277 (16)	1.500	5.41	78A,50A
3,0 2,0		49 879.179 (21)	3.000	1.66	
3,1 2,1		49 878.248 (21)	2.667	6.52	
3,2 2,2		49 875.455 (21)	1.667	21.10	
4,0 3,0		66 505.259 (24)	4.000	3.33	
4,1 3,1	66 503.98 (3)	66 504.018 (24)	3.750	8.19	78A
4,2 3,2		66 500.294 (24)	3.000	22.76	
4,3 3,3		66 494.090 (24)	1.750	47.05	
5,0 4,0		83 131.070 (24)	5.000	5.55	
5,1 4,1		83 129.519 (24)	4.800	10.40	
5,2 4,2		83 124.865 (23)	4.200	24.98	
5,3 4,3		83 117.110 (23)	3.200	49.27	
5,4 4,4		83 106.258 (26)	1.800	83.27	
6,0 5,0	99 756.55 (3)	99 756.545 (22)	6.000	8.32	78A
6,1 5,1	99 754.70 (3)	99 754.683 (21)	5.833	13.18	78A
6,2 5,2	99 749.10 (3)	99 749.099 (20)	5.333	27.75	78A
6,3 5,3	99 739.77 (3)	99 739.795 (20)	4.500	52.05	78A
6,4 5,4	99 726.79 (3)	99 726.774 (22)	3.333	86.04	78A
6,5 5,5	99 710.02 (3)	99 710.041 (29)	1.833	129.74	78A
7,0 6,0	116 381.65 (3)	116 381.616 (19)	7.000	11.65	78A
7,1 6,1	116 379.48 (3)	116 379.444 (18)	6.857	16.51	78A
7,2 6,2	116 372.96 (3)	116 372.930 (16)	6.429	31.08	78A
7,3 6,3	116 362.10 (3)	116 362.077 (15)	5.714	55.37	78A
7,4 6,4		116 346.888 (18)	4.714	89.37	
7,5 6,5		116 327.369 (26)	3.429	133.07	
7,6 6,6		116 303.529 (38)	1.857	186.45	
8,0 7,0	133 006.22 (3)	133 006.215 (20)	8.000	15.53	78A
8,1 7,1	133 003.74 (3)	133 003.734 (19)	7.875	20.39	78A
8,2 7,2	132 996.26 (3)	132 996.291 (17)	7.500	34.96	78A
8,3 7,3	132 983.87 (3)	132 983.889 (15)	6.875	59.25	78A
8,4 7,4	132 966.54 (3)	132 966.532 (17)	6.000	93.25	78A
8,5 7,5	132 944.31 (3)	132 944.229 (24)	4.875	136.95	78A
8,6 7,6	132 916.94 (3)	132 916.997 (37)	3.500	190.33	78A
8,7 7,7		132 884.818 (56)	1.875	253.39	
9,0 8,0	149 630.26 (3)	149 630.275 (27)	9.000	19.96	78A
9,1 8,1	149 627.46 (3)	149 627.484 (26)	8.889	24.82	78A
9,2 8,2	149 619.10 (3)	149 619.112 (24)	8.556	39.40	78A
9,3 8,3	149 605.14 (3)	149 605.162 (23)	8.000	63.69	78A
9,4 8,4	149 585.65 (3)	149 585.640 (23)	7.222	97.69	78A
9,5 8,5		149 560.553 (28)	6.222	141.38	
9,6 8,6	149 529.91 (3)	149 529.912 (37)	5.000	194.77	78A
9,7 8,7		149 493.728 (54)	3.556	257.83	
9,8 8,8		149 452.016 (02)	1.009	330.55	
10,0 9,0		166 253.728 (37)	10.000	24.96	
10,1 9,1		166 250.627 (36)	9.900	29.81	
10,2 9,2		166 241.327 (34)	9.600	44.39	
10,3 9,3		166 225.830 (33)	9.100	68.68	
10,4 9,4		166 204.143 (33)	8.400	102.68	
10,5 9,5		166 176.275 (35)	7.500	146.37	
10,6 9,6		166 142.236 (41)	6.400	199.75	
10,7 9,7		166 102.040 (53)	5.100	262.81	
10,8 9,8		166 055.703 (77)	3.600	335.53	
10,9 9,9		166 003.242 (120)	1.900	417.89	
11,0 10,0		182 876.503 (44)	11.000	30.50	
11,1 10,1		182 873.094 (43)	10.909	35.36	
11,2 10,2		182 862.865 (42)	10.636	49.94	
11,3 10,3		182 845.823 (40)	10.182	74.22	
11,4 10,4		182 821.973 (40)	9.545	108.22	
11,5 10,5		182 791.325 (42)	8.727	151.91	
11,6 10,6		182 753.890 (45)	7.727	205.30	
11,7 10,7		182 709.685 (52)	6.545	268.35	
11,8 10,8		182 658.726 (70)	5.182	341.07	
11,9 10,9		182 601.033 (110)	3.636	423.43	
11,10 10,10		182 536.629 (178)	1.909	515.41	
12,0 11,0		199 498.534 (45)	12.000	36.60	
12,1 11,1		199 494.815 (45)	11.917	41.46	
12,2 11,2		199 483.660 (43)	11.667	56.03	
12,3 11,3		199 465.073 (42)	11.250	80.32	
12,4 11,4		199 439.061 (42)	10.667	114.32	
12,5 11,5		199 405.635 (44)	9.917	158.01	
12,6 11,6		199 364.808 (46)	9.000	211.39	
12,7 11,7		199 316.596 (48)	7.917	274.45	
12,8 11,8		199 261.018 (59)	6.667	347.16	

TABLE 3 Microwave Spectrum of $^{13}\text{CH}_3\text{ }^{12}\text{C} \equiv ^{12}\text{CH}$ in the Ground Vibrational State (continued)

Transition $J'K' \leftarrow J''K''$	Obs. Freq. in MHz (Est. Unc.)	Calc. Freq. in MHz (Est. Unc.)	Line Strength	Approximate Energy in cm^{-1} Lower State	Ref.	
12,9	11,9	199 198.096 (95)	5.250	429.52		
12,10	11,10	199 127.855 (162)	3.667	521.49		
12,11	11,11	199 050.322 (268)	1.917	623.07		
13,0	12,0	216 119.751 (39)	13.000	43.26		
13,1	12,1	216 115.723 (38)	12.923	48.11		
13,2	12,2	216 103.641 (35)	12.692	62.69		
13,3	12,3	216 083.511 (34)	12.308	86.98		
13,4	12,4	216 055.339 (35)	11.769	120.97		
13,5	12,5	216 019.137 (39)	11.077	164.66		
13,6	12,6	215 974.920 (41)	10.231	218.04		
13,7	12,7	215 922.704 (41)	9.231	281.10		
13,8	12,8	215 862.511 (45)	8.077	353.81		
13,9	12,9	215 794.364 (75)	6.769	436.16		
13,10	12,10	215 718.290 (143)	5.308	528.14		
13,11	12,11	215 634.320 (251)	3.692	629.71		
13,12	12,12	215 542.486 (407)	1.923	740.85		
14,0	13,0	232 740.07 (3)	232 740.083 (39)	14.000	50.46	78A
14,1	13,1	232 735.78 (3)	232 735.747 (37)	13.929	55.32	78A
14,2	13,2	232 722.70 (3)	232 722.740 (32)	13.714	69.90	78A
14,3	13,3	232 701.07 (3)	232 701.067 (27)	13.357	94.18	78A
14,4	13,4	232 670.76 (3)	232 670.737 (29)	12.857	128.18	78A
14,5	13,5	232 631.81 (3)	232 631.762 (36)	12.214	171.87	78A
14,6	13,6	232 584.12 (3)	232 584.157 (42)	11.429	225.25	78A
14,7	13,7		232 527.942 (42)	10.500	288.30	
14,8	13,8	232 463.11 (3)	232 463.137 (40)	9.429	361.01	78A
14,9	13,9	232 389.79 (3)	232 389.770 (60)	8.214	443.36	78A
14,10	13,10		232 307.868 (125)	6.857	535.33	
14,11	13,11		232 217.465 (234)	5.357	636.90	
14,12	13,12		232 118.597 (394)	3.714	748.04	
14,13	13,13		232 011.302 (614)	1.929	868.73	
15,0	14,0	249 359.462 (79)	15.000	58.23		
15,1	14,1	249 354.817 (77)	14.933	63.09		
15,2	14,2	249 340.885 (73)	14.733	77.66		
15,3	14,3	249 317.672 (68)	14.400	101.95		
15,4	14,4	249 285.186 (68)	13.933	135.94		
15,5	14,5	249 243.440 (72)	13.333	179.63		
15,6	14,6	249 192.451 (78)	12.600	233.01		
15,7	14,7	249 132.239 (82)	11.733	296.06		
15,8	14,8	249 062.827 (81)	10.733	368.76		
15,9	14,9	248 984.244 (89)	9.600	451.11		
15,10	14,10	248 896.521 (133)	8.333	543.08		
15,11	14,11	248 799.691 (231)	6.933	644.65		
15,12	14,12	248 693.794 (309)	5.400	755.70		
15,13	14,13	248 578.872 (611)	3.733	876.46		
15,14	14,14	248 454.971 (910)	1.933	1006.66		
16,0	15,0	265 977.816 (164)	16.000	66.55		
16,1	15,1	265 972.864 (162)	15.937	71.40		
16,2	15,2	265 958.008 (158)	15.750	85.98		
16,3	15,3	265 933.255 (154)	15.437	110.26		
16,4	15,4	265 898.615 (151)	15.000	144.25		
16,5	15,5	265 854.101 (153)	14.437	187.94		
16,6	15,6	265 799.731 (157)	13.750	241.32		
16,7	15,7	265 735.527 (162)	12.937	304.37		
16,8	15,8	265 661.513 (166)	12.000	377.07		
16,9	15,9	265 577.719 (171)	10.937	459.42		
16,10	15,10	265 484.179 (196)	9.750	551.38		
16,11	15,11	265 380.929 (269)	8.437	652.94		
16,12	15,12	265 268.011 (408)	7.000	764.08		
16,13	15,13	265 145.469 (624)	5.437	884.76		
16,14	15,14	265 013.353 (924)	3.750	1014.95		
16,15	15,15	264 871.715 (1320)	1.937	1154.62		
17,0	16,0	282 595.075 (295)	17.000	75.42		
17,1	16,1	282 589.815 (294)	16.941	80.28		
17,2	16,2	282 574.037 (209)	16.765	94.05		
17,3	16,3	282 547.746 (284)	16.471	119.13		
17,4	16,4	282 510.954 (280)	16.059	153.12		
17,5	16,5	282 463.675 (279)	15.529	196.81		
17,6	16,6	282 405.928 (282)	14.882	250.18		
17,7	16,7	282 337.735 (288)	14.118	313.23		
17,8	16,8	282 259.124 (294)	13.235	385.93		
17,9	16,9	282 170.125 (301)	12.235	468.28		
17,10	16,10	282 070.774 (319)	11.118	560.24		
17,11	16,11	281 961.111 (369)	9.882	661.80		
17,12	16,12	281 841.179 (490)	8.529	772.93		
17,13	16,13	281 711.025 (674)	7.059	893.60		
17,14	16,14	281 570.703 (964)	5.471	1023.79		
17,15	16,15	281 420.267 (1359)	3.765	1163.46		
17,16	16,16	281 259.778 (1873)	1.941	1312.57		

TABLE 4 Microwave Spectrum of $^{12}\text{CH}_3$ $^{13}\text{C} \equiv ^{12}\text{CH}$ in the Ground Vibrational State

Transition $J'K' \leftarrow J''K''$	Obs. Freq. in MHz (Est. Unc.)	Calc. Freq. in MHz (Est. Unc.)	Line Strength	Approximate Energy in cm^{-1} Lower State	Ref.
1,0	0,0	17 084.652 (7)	1.000	0.00	
2,0	1,0	34 169.13 (10)	2.000	0.57	50A
2,1	1,1	34 168.47 (10)	1.500	5.42	50A
3,0	2,0	51 253.675 (17)	3.000	1.71	
3,1	2,1	51 252.698 (17)	2.667	6.56	
3,2	2,2	51 249.768 (17)	1.667	21.12	
4,0	3,0	68 337.905 (20)	4.000	3.42	
4,1	3,1	68 336.61 (3)	3.750	8.27	78A
4,2	3,2	68 332.72 (3)	3.000	22.82	78A
4,3	3,3	68 326.19 (3)	1.750	47.08	78A
5,0	4,0	85 421.852 (21)	5.000	5.70	
5,1	4,1	85 420.224 (20)	4.800	10.55	
5,2	4,2	85 415.340 (20)	4.200	25.10	
5,3	4,3	85 407.204 (19)	3.200	49.36	
5,4	4,4	85 395.817 (21)	1.800	83.30	
6,0	5,0	102 505.41 (3)	6.000	8.55	78A
6,1	5,1	102 503.46 (3)	5.833	13.40	78A
6,2	5,2	102 497.64 (3)	5.333	27.95	78A
6,3	5,3	102 487.86 (3)	4.500	52.21	78A
6,4	5,4	102 474.22 (3)	3.333	86.15	78A
6,5	5,5	102 456.65 (3)	1.833	129.78	78A
7,0	6,0	119 588.64 (3)	7.000	11.97	78A
7,1	6,1	119 586.37 (3)	6.857	16.82	78A
7,2	6,2	119 579.503 (16)	6.429	31.37	
7,3	6,3	119 568.11 (3)	5.714	55.62	78A
7,4	6,4	119 552.180 (17)	4.714	89.57	
7,5	6,5	119 531.700 (23)	3.429	133.20	
7,6	6,6	119 506.684 (34)	1.857	186.50	
8,0	7,0	136 671.34 (3)	8.000	15.96	78A
8,1	7,1	136 668.71 (3)	7.875	20.81	78A
8,2	7,2	136 660.87 (3)	7.500	35.36	78A
8,3	7,3	136 647.86 (3)	6.875	59.61	78A
8,4	7,4	136 629.64 (3)	6.000	93.56	78A
8,5	7,5	136 606.29 (3)	4.875	137.18	78A
8,6	7,6	136 577.67 (3)	3.500	190.49	78A
8,7	7,7	136 543.919 (47)	1.875	253.45	
9,0	8,0	153 753.37 (3)	9.000	20.51	78A
9,1	8,1	153 750.47 (3)	8.889	25.37	78A
9,2	8,2	153 741.68 (3)	8.556	39.92	78A
9,3	8,3	153 727.01 (3)	8.000	64.17	78A
9,4	8,4	153 706.59 (3)	7.222	98.11	78A
9,5	8,5	153 680.22 (3)	6.222	141.74	78A
9,6	8,6	153 648.06 (3)	5.000	195.04	78A
9,7	8,7	153 610.143 (42)	3.556	258.00	
9,8	8,8	153 566.372 (61)	1.889	330.61	
10,0	9,0	170 834.867 (25)	10.000	25.64	
10,1	9,1	170 831.615 (24)	9.900	30.49	
10,2	9,2	170 821.860 (22)	9.600	45.05	
10,3	9,3	170 805.606 (20)	9.100	69.30	
10,4	9,4	170 782.857 (19)	8.400	103.24	
10,5	9,5	170 753.623 (21)	7.500	146.87	
10,6	9,6	170 717.913 (27)	6.400	200.17	
10,7	9,7	170 675.741 (37)	5.100	263.13	
10,8	9,8	170 627.121 (52)	3.600	335.73	
10,9	9,9	170 572.070 (75)	1.900	417.96	
11,0	10,0	187 915.626 (26)	11.000	31.34	
11,1	10,1	187 912.050 (25)	10.909	36.19	
11,2	10,2	187 901.323 (23)	10.636	50.75	
11,3	10,3	187 883.449 (21)	10.182	75.00	
11,4	10,4	187 858.433 (21)	9.545	108.94	
11,5	10,5	187 826.286 (22)	8.727	152.56	
11,6	10,6	187 787.018 (25)	7.727	205.86	
11,7	10,7	187 740.644 (30)	6.545	268.82	
11,8	10,8	187 687.179 (39)	5.182	341.42	
11,9	10,9	187 626.643 (58)	3.636	423.65	
11,10	10,10	187 559.057 (91)	1.909	515.48	
12,0	11,0	204 995.65 (3)	12.000	37.61	78A
12,1	11,1	204 991.68 (3)	11.917	42.46	78A
12,2	11,2	204 980.07 (3)	11.667	57.01	78A
12,3	11,3	204 960.52 (3)	11.250	81.26	78A
12,4	11,4	204 933.24 (3)	10.667	115.20	78A
12,5	11,5	204 898.17 (3)	9.917	158.83	78A
12,6	11,6	204 855.33 (3)	9.000	212.12	78A
12,7	11,7	204 804.779 (24)	7.917	275.08	

TABLE 4 Microwave Spectrum of $^{12}\text{CH}_3\ ^{13}\text{C} \equiv ^{12}\text{CH}$ in the Ground Vibrational State (continued).

Transition $J'K' \leftarrow J''K''$		Obs. Freq. in MHz (Est. Unc.)	Calc. Freq. in MHz (Est. Unc.)	Line Strength	Approximate Energy in cm^{-1} Lower State	Ref.
12,8	11,8	204 746.49 (3)	204 746.475 (26)	6.667	347.68	78A
12,9	11,9	204 680.53 (3)	204 680.459 (37)	5.250	429.90	78A
12,10	11,10		204 606.755 (68)	2.667	521.74	
12,11	11,11		204 525.389 (120)	1.917	623.15	
13,0	12,0	222 074.70 (3)	222 074.723 (26)	13.000	44.45	78A
13,1	12,1	222 070.52 (3)	222 070.500 (25)	12.923	49.30	78A
13,2	12,2	222 057.79 (3)	222 057.832 (23)	12.692	63.85	78A
13,3	12,3	222 036.66 (3)	222 036.723 (20)	12.308	88.10	78A
13,4	12,4		222 007.181 (21)	11.769	122.04	
13,5	12,5	221 969.18 (3)	221 969.217 (26)	11.077	165.66	78A
13,6	12,6	221 922.88 (3)	221 922.843 (31)	10.231	218.96	78A
13,7	12,7	221 868.10 (3)	221 868.077 (33)	9.231	281.91	78A
13,8	12,8	221 804.98 (3)	221 804.938 (32)	8.077	354.51	78A
13,9	12,9	221 733.38 (3)	221 733.448 (33)	6.769	436.73	78A
13,10	12,10	221 653.61 (3)	221 653.633 (55)	5.308	528.56	78A
13,11	12,11		221 565.520 (104)	3.692	629.97	
13,12	12,12		221 469.143 (181)	1.923	740.94	
14,0	13,0	239 152.94 (3)	239 152.915 (50)	14.000	51.86	78A
14,1	13,1		239 140.369 (50)	13.929	56.71	
14,2	13,2		239 134.732 (47)	13.714	71.26	
14,3	13,3		239 112.009 (46)	13.357	95.51	
14,4	13,4		239 080.207 (47)	12.857	129.45	
14,5	13,5		239 039.340 (52)	12.214	173.07	
14,6	13,6		238 989.420 (58)	11.429	226.36	
14,7	13,7		238 930.465 (65)	10.500	289.31	
14,8	13,8		238 862.497 (69)	9.429	361.91	
14,9	13,9		238 785.540 (73)	8.214	444.13	
14,10	13,10		238 699.621 (85)	6.857	535.95	
14,11	13,11		238 604.770 (119)	5.357	637.36	
14,12	13,12		238 501.022 (187)	3.714	748.32	
14,13	13,13		238 388.413 (291)	1.929	868.82	
15,0	14,0		256 230.105 (102)	15.000	59.83	
15,1	14,1		256 225.236 (101)	14.933	64.68	
15,2	14,2		256 210.631 (100)	14.733	79.23	
15,3	14,3		256 186.296 (98)	14.400	103.48	
15,4	14,4		256 152.238 (99)	13.933	137.42	
15,5	14,5		256 108.471 (103)	13.333	181.04	
15,6	14,6		256 055.009 (111)	12.600	234.33	
15,7	14,7		255 991.871 (120)	11.733	297.28	
15,8	14,8		255 919.081 (131)	10.733	369.00	
15,9	14,9		255 836.663 (141)	9.600	452.09	
15,10	14,10		255 744.648 (155)	8.333	543.92	
15,11	14,11		255 643.068 (183)	6.933	645.32	
15,12	14,12		255 531.959 (236)	5.400	756.28	
15,13	14,13		255 411.361 (329)	3.733	876.77	
15,14	14,14		255 281.317 (467)	1.933	1006.76	
16,0	15,0		273 306.218 (185)	16.000	68.38	
16,1	15,1		273 301.027 (184)	15.937	73.23	
16,2	15,2		273 285.456 (182)	15.750	87.78	
16,3	15,3		273 259.510 (180)	15.437	112.03	
16,4	15,4		273 223.200 (180)	15.000	145.96	
16,5	15,5		273 176.536 (183)	14.437	189.58	
16,6	15,6		273 119.537 (191)	13.750	242.87	
16,7	15,7		273 052.223 (204)	12.937	305.82	
16,8	15,8		272 974.617 (219)	12.000	378.41	
16,9	15,9		272 888.747 (237)	10.937	460.63	
16,10	15,10		272 788.644 (258)	9.750	552.45	
16,11	15,11		272 680.343 (287)	8.437	653.85	
16,12	15,12		272 561.883 (336)	7.000	764.80	
16,13	15,13		272 433.307 (417)	5.437	885.29	
16,14	15,14		272 294.660 (543)	3.750	1015.27	
16,15	15,15		272 145.992 (725)	1.937	1154.72	
17,0	16,0		290 381.180 (305)	17.000	77.50	
17,1	16,1		290 375.667 (304)	16.941	82.35	
17,2	16,2		290 359.131 (301)	16.765	96.90	
17,3	16,3		290 331.578 (299)	16.471	121.14	
17,4	16,4		290 293.018 (298)	16.059	155.08	
17,5	16,5		290 243.463 (300)	15.529	198.70	
17,6	16,6		290 182.932 (308)	14.882	251.98	
17,7	16,7		290 111.447 (322)	14.118	314.93	
17,8	16,8		290 029.032 (342)	13.235	387.52	
17,9	16,9		289 935.717 (366)	12.235	469.73	
17,10	16,10		289 831.536 (395)	11.118	561.55	
17,11	16,11		289 716.525 (432)	9.882	662.94	
17,12	16,12		289 590.726 (484)	8.529	773.89	
17,13	16,13		289 454.183 (561)	7.059	894.38	
17,14	16,14		289 306.946 (678)	5.471	1024.35	
17,15	16,15		289 149.067 (848)	3.765	1163.80	
17,16	16,16		288 980.603 (1085)	1.941	1312.68	

TABLE 5 Microwave Spectrum of $^{12}\text{CH}_3 - ^{12}\text{C} = ^{13}\text{CH}$ in the Ground Vibrational State.

Transition $J'K' \leftarrow J''K''$	Obs. Freq. in MHz (Est. Unc.)	Calc. Freq. in MHz (Est. Unc.)	Line Strength	Approximate Energy in cm^{-1} Lower State	Ref.
1,0 0,0		16 580.488 (6)	1.000	0.00	
2,0 1,0	33 160.94 (3)	33 160.910 (12)	2.000	0.55	78A,50A
2,1 1,1	33 160.35 (3)	33 160.288 (12)	1.500	5.41	78A,50A
3,0 2,0		49 741.197 (16)	3.000	1.66	
3,1 2,1		49 740.263 (16)	2.667	6.52	
3,2 2,2		49 737.465 (16)	1.667	21.10	
4,0 3,0		66 321.282 (19)	4.000	3.32	
4,1 3,1	66 320.01 (3)	66 320.038 (19)	3.750	8.18	78A
4,2 3,2		66 316.307 (18)	3.000	22.76	
4,3 3,3	66 310.05 (3)	66 310.089 (18)	1.750	47.05	78A
5,0 4,0		82 901.100 (20)	5.000	5.53	
5,1 4,1		82 899.545 (19)	4.800	10.39	
5,2 4,2		82 894.881 (19)	4.200	24.97	
5,3 4,3		82 887.110 (19)	3.200	49.26	
5,4 4,4		82 876.235 (21)	1.800	83.27	
6,0 5,0	99 480.52 (3)	99 480.583 (19)	6.000	8.30	78A
6,1 5,1	99 478.69 (3)	99 478.718 (18)	5.833	13.16	78A
6,2 5,2	99 473.07 (3)	99 473.122 (17)	5.333	27.73	78A
6,3 5,3	99 463.77 (3)	99 463.797 (17)	4.500	52.03	78A
6,4 5,4	99 450.75 (3)	99 450.749 (19)	3.333	86.03	78A
6,5 5,5	99 433.95 (3)	99 433.982 (25)	1.833	129.74	78A
7,0 6,0	116 059.70 (3)	116 059.667 (18)	7.000	11.61	78A
7,1 6,1	116 057.53 (3)	116 057.490 (17)	6.857	16.47	78A
7,2 6,2	116 051.01 (3)	116 050.962 (15)	6.429	31.05	78A
7,3 6,3	116 040.13 (3)	116 040.086 (14)	5.714	55.35	78A
7,4 6,4		116 024.864 (16)	4.714	89.35	
7,5 6,5		116 005.306 (23)	3.429	133.05	
7,6 6,6		115 981.418 (36)	1.857	186.45	
8,0 7,0	132 638.26 (3)	132 638.284 (19)	8.000	15.48	78A
8,1 7,1	132 635.91 (3)	132 635.790 (10)	7.875	20.34	78A
8,2 7,2	132 628.35 (3)	132 628.338 (16)	7.500	34.92	78A
8,3 7,3	132 615.92 (3)	132 615.909 (14)	6.875	59.22	78A
8,4 7,4	132 598.52 (3)	132 598.516 (15)	6.000	93.22	78A
8,5 7,5	132 576.16 (3)	132 576.167 (22)	4.875	136.92	78A
8,6 7,6	132 548.86 (3)	132 548.870 (34)	3.500	190.32	78A
8,7 7,7		132 516.639 (53)	1.875	253.39	
9,0 8,0	149 216.35 (3)	149 216.372 (22)	9.000	19.91	78A
9,1 8,1	149 213.55 (3)	149 213.574 (21)	8.889	24.77	78A
9,2 8,2	149 205.18 (3)	149 205.184 (19)	8.556	39.35	78A
9,3 8,3	149 191.26 (3)	149 191.204 (17)	8.000	63.64	78A
9,4 8,4	149 171.62 (3)	149 171.640 (17)	7.222	97.64	78A
9,5 8,5	149 146.51 (3)	149 146.501 (22)	6.222	141.35	78A
9,6 8,6	149 115.84 (3)	149 115.798 (33)	5.000	194.74	78A
9,7 8,7		149 079.544 (50)	3.556	257.81	
9,8 8,8		149 037.754 (77)	1.889	330.54	
10,0 9,0		165 793.864 (27)	10.000	24.89	
10,1 9,1		165 790.757 (26)	9.900	29.75	
10,2 9,2		165 781.436 (24)	9.600	44.32	
10,3 9,3		165 765.905 (22)	9.100	68.62	
10,4 9,4		165 744.172 (21)	8.400	102.62	
10,5 9,5		165 716.245 (24)	7.500	146.32	
10,6 9,6		165 682.137 (32)	6.400	199.71	
10,7 9,7		165 641.862 (46)	5.100	262.78	
10,8 9,8		165 595.438 (72)	3.600	335.51	
10,9 9,9		165 542.884 (113)	1.900	417.88	
11,0 10,0		182 370.699 (30)	11.000	30.42	
11,1 10,1		182 367.281 (29)	10.909	35.28	
11,2 10,2		182 357.031 (27)	10.636	49.85	
11,3 10,3		182 339.951 (26)	10.182	74.15	
11,4 10,4		182 316.049 (25)	9.545	108.15	
11,5 10,5		182 285.336 (27)	8.727	151.85	
11,6 10,6		182 247.825 (31)	7.727	205.24	
11,7 10,7		182 203.532 (41)	6.545	268.31	
11,8 10,8		182 152.476 (64)	5.182	341.03	
11,9 10,9		182 094.679 (104)	3.636	423.40	
11,10 10,10		182 030.166 (166)	1.909	515.40	
12,0 11,0		198 946.813 (30)	12.000	36.50	
12,1 11,1		198 943.086 (24)	11.917	41.36	
12,2 11,2		198 931.906 (27)	11.667	55.94	
12,3 11,3		198 913.277 (25)	11.250	80.23	
12,4 11,4		198 887.209 (25)	10.667	114.23	
12,5 11,5		198 853.712 (26)	9.917	157.93	
12,6 11,6		198 812.800 (28)	9.000	211.32	
12,7 11,7		198 764.491 (34)	7.917	274.38	
12,8 11,8		198 708.807 (51)	6.667	347.11	
12,9 11,9		198 645.770 (89)	5.250	429.48	

MICROWAVE SPECTRUM OF PROPYNE

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TABLE 5 Microwave Spectrum of $^{12}\text{CH}_3\ ^{12}\text{C} \equiv ^{13}\text{CH}$ in the Ground Vibrational State (continued).

Transition $J'K' \leftarrow J''K''$	Obs. Freq. in MHz (Est. Unc.)	Calc. Freq. in MHz (Est. Unc.)	Line Strength	Approximate Energy in cm^{-1} Lower State	Ref.
12,10 11,10		198 575.409 (153)	3.667	521.47	
12,11 11,11		198 497.753 (248)	1.917	623.06	
13,0 12,0	215 522.17 (3)	215 522.145 (23)	13.000	43.14	78A
13,1 12,1	215 518.12 (3)	215 518.108 (24)	12.923	48.00	78A
13,2 12,2	215 505.96 (3)	215 505.999 (21)	12.692	62.57	78A
13,3 12,3	215 485.82 (3)	215 485.824 (19)	12.308	86.86	78A
13,4 12,4	215 457.58 (3)	215 457.590 (20)	11.769	120.86	78A
13,5 12,5	215 421.31 (3)	215 421.310 (23)	11.077	164.56	78A
13,6 12,6	215 376.95 (3)	215 377.000 (25)	10.231	217.95	78A
13,7 12,7	215 324.65 (3)	215 324.679 (26)	9.231	281.01	78A
13,8 12,8		215 264.370 (56)	8.077	353.74	
13,9 12,9		215 196.097 (71)	6.769	436.10	
13,10 12,10		215 119.892 (135)	5.308	528.09	
13,11 12,11		215 035.786 (233)	3.692	629.68	
13,12 12,12		214 943.817 (370)	1.923	740.84	
14,0 13,0	232 096.61 (3)	232 096.634 (32)	14.000	50.33	78A
14,1 13,1	232 092.26 (3)	232 092.288 (30)	13.929	55.18	78A
14,2 13,2	232 079.26 (3)	232 079.251 (27)	13.714	69.75	78A
14,3 13,3	232 057.54 (3)	232 057.529 (24)	13.357	94.05	78A
14,4 13,4	232 027.20 (3)	232 027.132 (25)	12.857	128.05	78A
14,5 13,5		231 998.072 (30)	12.214	171.75	
14,6 13,6	231 940.37 (3)	231 940.367 (33)	11.429	225.13	78A
14,7 13,7	231 884.04 (3)	231 884.037 (32)	10.500	288.20	78A
14,8 13,8	231 819.11 (3)	231 819.105 (32)	9.429	360.92	78A
14,9 13,9	231 745.61 (3)	231 745.601 (58)	8.214	443.28	78A
14,10 13,10		231 663.556 (119)	6.857	535.27	
14,11 13,11		231 573.006 (217)	5.357	636.05	
14,12 13,12		231 473.989 (357)	3.714	748.01	
14,13 13,13		231 366.549 (549)	1.929	868.72	
15,0 14,0		248 670.221 (68)	15.000	58.07	
15,1 14,1		248 665.566 (67)	14.933	62.93	
15,2 14,2		248 651.602 (64)	14.733	77.50	
15,3 14,3		248 628.335 (61)	14.400	101.79	
15,4 14,4		248 595.776 (61)	13.933	135.79	
15,5 14,5		248 553.939 (64)	13.333	179.49	
15,6 14,6		248 502.841 (68)	12.600	232.87	
15,7 14,7		248 442.505 (69)	11.733	295.93	
15,8 14,8		248 372.956 (68)	10.733	368.65	
15,9 14,9		248 294.224 (77)	9.600	451.01	
15,10 14,10		248 206.345 (120)	8.333	543.00	
15,11 14,11		248 109.355 (210)	6.933	644.58	
15,12 14,12		248 003.297 (349)	5.400	755.73	
15,13 14,13		247 888.217 (544)	3.733	876.43	
15,14 14,14		247 764.164 (803)	1.933	1006.65	
16,0 15,0		265 242.847 (135)	16.000	66.36	
16,1 15,1		265 237.883 (133)	15.937	71.22	
16,2 15,2		265 222.993 (131)	15.750	85.80	
16,3 15,3		265 198.183 (127)	15.437	110.09	
16,4 15,4		265 163.464 (124)	15.000	144.08	
16,5 15,5		265 118.852 (127)	14.437	187.78	
16,6 15,6		265 064.364 (130)	13.750	241.16	
16,7 15,7		265 000.026 (133)	12.937	304.22	
16,8 15,8		264 925.863 (134)	12.000	376.94	
16,9 15,9		264 841.910 (139)	10.937	459.30	
16,10 15,10		264 748.201 (163)	9.750	551.27	
16,11 15,11		264 644.777 (232)	8.437	652.85	
16,12 15,12		264 531.685 (358)	7.000	764.01	
16,13 15,13		264 408.971 (548)	5.437	884.70	
16,14 15,14		264 276.690 (810)	3.750	1014.91	
16,15 15,15		264 134.900 (1153)	1.937	1154.61	
17,0 16,0		281 814.455 (234)	17.000	75.21	
17,1 16,1		281 809.183 (233)	16.941	80.07	
17,2 16,2		281 793.367 (229)	16.765	94.64	
17,3 16,3		281 767.016 (225)	16.471	118.93	
17,4 16,4		281 730.139 (222)	16.059	152.93	
17,5 16,5		281 682.754 (222)	15.529	196.62	
17,6 16,6		281 624.881 (224)	14.882	250.00	
17,7 16,7		281 556.543 (228)	14.118	313.06	
17,8 16,8		281 477.772 (232)	13.235	385.77	
17,9 16,9		281 398.601 (237)	12.235	468.13	
17,10 16,10		281 289.069 (253)	11.118	560.11	
17,11 16,11		281 179.219 (301)	9.882	661.68	
17,12 16,12		281 059.098 (404)	8.529	772.83	
17,13 16,13		280 928.758 (578)	7.059	893.52	
17,14 16,14		280 788.257 (813)	5.471	1023.73	
17,15 16,15		280 637.656 (1178)	3.765	1163.42	
17,16 16,16		280 477.020 (1623)	1.941	1312.56	

TABLE 6. Molecular constants for $\text{CH}_3\text{C}\equiv\text{CH}$ (v_{10} vibrational state)

B^*	= 8569.9875 (17) MHz
D_J	= 2.966 (22) kHz
D_{JK}	= 163.780 (57) kHz
ρ^*	= 1.97 (22) kHz
q	= 4.1938 (6) MHz
ζ_{10}	= 0.892 (1) ^a

^a Derived with data from reference [73A]: $A_0 = 158620$ MHz (calculated from the structure).

Table 7 : Microwave spectrum of $\text{CH}_3\text{C} \equiv \text{CH}$ in the ν_{10} vibrational state

Transition J' J''	K	ℓ	Observed frequency (Estimated uncertainty)	Calculated frequency (Estimated uncertainty)	Line Strength	Reference
1 - 0	0	± 1		17 139.623 (3)	1.0	
2 - 1	± 1	± 1	34 313.21 (10)	34 313.405 (7)	1.5	50A
	0	± 1	34 278.98 (10)	34 279.126 (6)	2.0	50A
	± 1	∓ 1	34 277.05 (10)	34 277.186 (6)	1.5	50A
	± 1	± 1	34 246.30 (10)	34 246.305 (7)	1.5	50A
3 - 2	± 1	± 1	51 469.85 (10)	51 469.930 (10)	2.7	50A
	± 2	± 1	51 418.75 (10)	51 418.855 (8)	1.7	50A
	0	± 1	51 418.23 (10)	51 418.388 (8)	3.0	50A
	± 1	∓ 1	51 415.35 (10)	51 415.540 (8)	2.7	50A
	± 2	∓ 1	51 410.51 (10)	51 410.651 (8)	1.7	50A
	± 1	± 1	51 369.12 (10)	51 369.279 (10)	2.7	50A
4 - 3	± 1	± 1	68 626.217 (30)	68 626.241 (13)	3.7	69A
	± 2	± 1	68 558.447 (30)	68 558.371 (9)	3.0	69A
	0	± 1	68 557.333 (30)	68 557.290 (9)	4.0	69A
	± 3	± 1	68 554.251 (30)	68 554.194 (9)	1.7	69A
	± 1	∓ 1	68 553.602 (30)	68 553.606 (9)	3.7	69A
	± 2	∓ 1	68 547.148 (30)	68 547.127 (9)	3.0	69A
	± 3	∓ 1	68 538.052 (30)	68 537.982 (10)	1.7	69A
	± 1	± 1	68 491.993 (30)	68 492.040 (13)	3.7	69A
5 - 4	± 1	± 1	85 782.322 (60)	85 782.268 (14)	4.8	69A
	± 2	± 1	85 697.750 (60)	85 697.799 (10)	4.2	69A
	0	± 1	85 695.638 (60)	85 695.709 (10)	5	69A
	± 3	± 1	85 692.374 (60)	85 692.393 (9)	3.2	69A
	± 1	∓ 1	85 691.206 (60)	85 691.289 (8)	4.8	69A
	± 4	± 1	85 684.002 (60)	85 684.051 (11)	1.8	69A
	± 2	∓ 1	85 683.174 (60)	85 683.256 (9)	4.2	69A
	± 3	∓ 1		85 671.852 (10)	3.2	
	± 4	∓ 1		85 657.143 (13)	1.8	
	± 1	± 1	85 614.570 (60)	85 614.516 (14)	4.8	69A
6 - 5	± 1	± 1	102 938.040 (90)	102 937.938 (16)	5.8	69A
	± 2	± 1	102 837.186 (90)	102 837.117 (15)	5.3	69A
	0	± 1	102 833.604 (90)	102 833.526 (14)	6	69A
	± 3	± 1	102 830.418 (90)	102 830.359 (9)	4.5	69A
	± 1	∓ 1	102 828.543 (90)	102 828.492 (9)	5.8	69A
	± 4	± 1	102 820.305 (90)	102 820.261 (10)	3.3	69A
	± 2	∓ 1	102 818.949 (90)	102 818.937 (8)	5.3	69A
	± 5	± 1	102 806.442 (90)	102 806.379 (15)	1.8	69A
	± 3	∓ 1	102 805.311 (90)	102 805.304 (9)	4.5	69A
	± 4	∓ 1	102 787.743 (90)	102 787.682 (13)	3.3	69A
	± 5	∓ 1	102 766.158 (90)	102 766.097 (18)	1.8	69A
	± 1	± 1	102 736.692 (90)	102 736.636 (16)	5.8	69A
7 - 6	± 1	± 1	120 093.174 (60)	120 093.181 (21)	6.9	69A
	± 2	± 1	119 976.230 (60)	119 976.304 (24)	6.4	69A
	0	± 1	119 970.604 (60)	119 970.621 (23)	7.0	69A
	± 3	± 1	119 968.032 (60)	119 968.046 (14)	5.7	69A
	± 1	∓ 1	119 965.098 (60)	119 965.121 (14)	6.9	69A
	± 4	± 1	119 956.112 (60)	119 956.139 (13)	4.7	69A
	± 2	∓ 1	119 954.032 (60)	119 954.099 (12)	6.4	69A
	± 5	± 1	119 939.884 (60)	119 939.882 (17)	3.4	69A
	± 3	∓ 1	119 938.214 (60)	119 938.255 (13)	5.7	69A
	± 6	± 1	119 919.060 (60)	119 919.132 (24)	1.8	69A

TABLE 7 : Microwave Spectrum of $\text{CH}_3\text{C} \equiv \text{CH}$ in the ν_{10} Vibrational State (continued)

Transition J' J''	K	ℓ	Observed frequency (Estimated uncertainty)	Calculated frequency (Estimated uncertainty)	Line Strength	Reference
8 - 7	± 4	∓ 1	119 917.696 (60)	119 917.732 (16)	4.7	69A
	± 5	∓ 1	119 892.576 (60)	119 892.577 (21)	3.4	69A
	± 6	∓ 1		119 862.807 (29)	1.8	
	± 1	± 1	119 858.368 (60)	119 858.329 (21)	6.9	69A
	± 1	± 1		137 247.926 (30)	7.8	
	± 2	± 1		137 115.336 (39)	7.5	
	0	± 1		137 106.873 (37)	8	
	± 3	± 1		137 105.406 (25)	6.9	
	± 1	∓ 1		137 101.080 (25)	7.9	
	± 4	± 1		137 091.634 (22)	6.0	
	± 2	∓ 1		137 088.647 (23)	7.5	
	± 5	± 1		137 072.974 (24)	4.9	
	± 3	∓ 1		137 070.621 (22)	6.9	
	± 6	± 1		137 049.210 (30)	3.5	
	± 4	∓ 1		137 047.216 (23)	6.0	
	± 7	± 1		137 020.276 (39)	1.9	
	± 5	∓ 1		137 018.499 (27)	4.9	
	± 6	∓ 1		136 984.501 (34)	3.5	
9 - 8	± 1	∓ 1		136 979.524 (30)	7.9	
	± 7	∓ 1		136 945.236 (44)	1.9	
	± 1	± 1		154 402.102 (44)	8.9	
	± 2	± 1		154 254.193 (60)	8.6	
	± 3	± 1		154 242.394 (42)	8.0	
	0	± 1		154 242.161 (56)	9.0	
	± 1	∓ 1		154 236.272 (42)	8.9	
	± 4	± 1		154 226.693 (37)	7.2	
	± 2	∓ 1		154 222.493 (38)	8.6	
	± 5	± 1		154 205.594 (37)	6.2	
	± 3	∓ 1		154 202.319 (37)	8.0	
	± 6	± 1		154 178.797 (40)	5.0	
	± 4	∓ 1		154 176.051 (37)	7.2	
	± 7	± 1		154 146.205 (48)	3.6	
	± 5	∓ 1		154 143.786 (39)	6.2	
	± 8	± 1		154 107.773 (60)	1.9	
	± 6	∓ 1		154 105.560 (45)	5.0	
10 - 9	± 1	∓ 1		154 100.149 (44)	8.9	
	± 7	∓ 1		154 061.419 (54)	3.6	
	± 8	∓ 1		154 011.349 (66)	1.9	
	± 1	± 1		171 555.636 (64)	9.9	
	± 2	± 1		171 392.852 (87)	9.6	
	± 3	± 1		171 378.963 (65)	9.1	
	0	± 1		171 376.366 (62)	10.0	
	± 1	∓ 1		171 370.601 (63)	9.9	
	± 4	± 1		171 361.256 (58)	8.4	
	± 2	∓ 1		171 355.552 (59)	9.6	
	± 5	± 1		171 337.684 (56)	7.5	
	± 3	∓ 1		171 333.266 (57)	9.1	
	± 6	± 1		171 307.832 (58)	6.4	

TABLE 7 : Microwave Spectrum of $\text{CH}_3\text{C} \equiv \text{CH}$ in the ν_{10} Vibrational State (continued)

Transition J'	J''	K	ξ	Observed frequency (Estimated uncertainty)	Calculated frequency (Estimated uncertainty)	Line Strength	Reference
11 - 10	± 4	∓ 1			171 304.156 (56)	8.4	
	± 7	± 1			171 271.565 (63)	5.1	
	± 5	∓ 1			171 268.360 (57)	7.5	
	± 8	± 1			171 228.827 (73)	3.6	
	± 6	∓ 1			171 225.932 (61)	6.4	
	± 1	± 1			171 220.133 (64)	9.9	
	± 9	± 1			171 179.587 (87)	1.9	
	± 7	∓ 1			171 176.904 (68)	5.1	
	± 8	∓ 1			171 121.294 (79)	3.6	
	± 9	∓ 1			171 059.109 (94)	1.9	
	± 1	± 1			188 708.459 (90)	10.9	
	± 2	± 1			188 531.291 (121)	10.6	
	± 3	± 1			188 515.065 (93)	10.2	
	0	± 1			188 509.367 (114)	11.0	
	± 1	∓ 1			188 503.973 (91)	10.9	
	± 4	± 1			188 495.272 (85)	9.6	
	± 2	∓ 1			188 487.735 (86)	10.6	
12 - 11	± 5	± 1			188 469.185 (82)	8.7	
	± 3	∓ 1			188 463.378 (83)	10.2	
	± 6	± 1			188 436.252 (81)	7.7	
	± 4	∓ 1			188 431.453 (82)	9.6	
	± 7	± 1			188 396.297 (84)	6.5	
	± 5	∓ 1			100 392.130 (01)	0.7	
	± 8	± 1			188 349.239 (92)	5.2	
	± 6	∓ 1			188 345.514 (84)	7.7	
	± 1	± 1			188 339.405 (90)	10.9	
	± 9	± 1			188 295.040 (104)	3.6	
	± 7	∓ 1			188 291.618 (89)	6.5	
	± 10	± 1			188 233.678 (121)	1.9	
	0	∓ 1			188 230.472 (98)	5.2	
	± 9	∓ 1			188 162.090 (112)	3.6	
	± 10	∓ 1			188 086.478 (129)	1.9	
	± 1	± 1			205 860.498 (122)	11.9	
	± 2	± 1			205 669.488 (163)	11.7	
	± 3	± 1			205 650.656 (128)	11.3	
	0	± 1			205 641.043 (153)	12.0	
	± 1	∓ 1			205 636.291 (124)	11.9	
	± 4	± 1			205 628.687 (118)	10.7	
	± 2	∓ 1			205 618.952 (118)	11.7	
	± 5	± 1			205 600.038 (113)	9.9	
	± 3	∓ 1			205 592.571 (115)	11.3	
	± 6	± 1			205 563.999 (111)	9.0	
	± 4	∓ 1			205 557.857 (113)	10.7	
	± 7	± 1			205 520.337 (113)	7.9	
	± 5	∓ 1			205 515.043 (112)	9.9	
	± 8	± 1			205 468.946 (118)	6.7	
	± 6	∓ 1			205 464.235 (113)	9.0	
	± 1	± 1			205 457.894 (122)	11.9	
	± 9	± 1			205 409.780 (128)	5.2	
	± 7	∓ 1			205 405.479 (116)	7.9	
	± 10	± 1			205 342.808 (143)	3.7	

TABLE 7 : Microwave Spectrum of $\text{CH}_3\text{C}\equiv\text{CH}$ in the v_{10} Vibrational State (continued)

Transition J'	J''	K	ℓ	Observed frequency (Estimated uncertainty)	Calculated frequency (Estimated uncertainty)	Line Strength	Reference
13 - 12	±8	±1			205 338.806 (124)	6.7	
	±11	±1			205 268.014 (163)	1.9	
	±9	±1			205 264.232 (135)	5.2	
	±10	±1			205 181.769 (152)	3.7	
	±11	±1			205 091.421 (173)	1.9	
	±1	±1			223 011.683 (160)	12.9	
	±2	±1			222 807.422 (213)	12.7	
	±3	±1			222 785.687 (170)	12.3	
	0	±1			222 771.274 (200)	13.0	
	±1	±1			222 767.459 (165)	12.9	
	±4	±1			222 761.442 (158)	11.8	
	±2	±1			222 749.121 (157)	12.7	
	±5	±1			222 730.184 (152)	11.1	
	±3	±1			222 720.762 (154)	12.3	
	±6	±1			222 691.009 (149)	10.2	
	±4	±1			222 683.289 (151)	11.8	
	±7	±1			222 643.618 (148)	9.2	
	±5	±1			222 636.997 (149)	11.1	
	±8	±1			222 587.883 (152)	8.1	
	±6	±1			222 582.017 (149)	10.2	
	±1	±1			222 575.529 (160)	12.9	
	±9	±1			222 523.738 (159)	6.8	
	±7	±1			222 518.413 (151)	9.2	
	±10	±1			222 451.148 (172)	5.3	
	±8	±1			222 446.221 (156)	8.1	
	±11	±1			222 370.091 (190)	3.7	
	±9	±1			222 365.463 (166)	6.8	
	±12	±1			222 280.554 (213)	1.9	
	±10	±1			222 276.152 (180)	5.3	
	±11	±1			222 178.295 (200)	3.7	
	±12	±1			222 071.901 (224)	1.9	
14 - 13	±1	±1			240 161.943 (206)	13.9	
	±2	±1			239 945.070 (271)	13.7	
	±3	±1			239 920.113 (219)	13.4	
	0	±1			239 899.939 (255)	14.0	
	±1	±1			239 897.382 (212)	13.9	
	±4	±1			239 893.486 (205)	12.9	
	±2	±1			239 878.150 (203)	13.7	
	±5	±1			239 859.565 (198)	12.2	
	±3	±1			239 847.868 (199)	13.4	
	±6	±1			239 817.222 (193)	11.4	
	±4	±1			239 807.666 (196)	12.9	
	±7	±1			239 766.082 (192)	10.5	
	±5	±1			239 757.917 (193)	12.2	
	±8	±1			239 705.986 (193)	9.4	
	±6	±1			239 698.781 (192)	11.4	
	±1	±1			239 692.238 (206)	13.9	
	±9	±1			239 636.852 (198)	8.2	
	±7	±1			239 630.340 (193)	10.5	
	±10	±1			239 558.634 (209)	6.9	
	±8	±1			239 552.639 (197)	9.4	
	±11	±1			239 471.307 (224)	5.4	
	±9	±1			239 374.855 (245)	8.2	

TABLE 7 : Microwave Spectrum of $\text{CH}_3\text{C} \equiv \text{CH}$ in the ν_{10} Vibrational State (continued)

Transition J' J''	K	ℓ	Observed frequency (Estimated uncertainty)	Calculated frequency (Estimated uncertainty)	Line Strength	Reference
15 - 14	±12	±1		239 374.855 (245)	3.7	
	±10	±1		239 369.550 (217)	6.9	
	±13	±1		239 269.265 (272)	1.9	
	±11	±1		239 264.190 (234)	5.4	
	±12	±1		239 149.632 (257)	3.7	
	±13	±1		239 025.882 (285)	1.9	
	±1	±1		257 311.205 (259)	14.9	
	±2	±1		257 082.410 (339)	14.7	
	±3	±1		257 053.886 (277)	14.4	
	0	±1		257 026.919 (319)	15.0	
	±1	±1		257 025.963 (268)	14.9	
	±4	±1		257 024.764 (260)	13.9	
	±2	±1		257 005.951 (257)	14.7	
	±5	±1		256 988.122 (251)	13.3	
	±3	±1		256 973.805 (252)	14.4	
	±6	±1		256 942.576 (246)	12.6	
	±4	±1		256 930.909 (249)	13.9	
	±7	±1		256 887.665 (243)	11.7	
	±5	±1		256 877.726 (245)	13.3	
	±8	±1		256 823.189 (242)	10.7	
	±6	±1		256 814.452 (243)	12.6	
	±1	±1		256 807.951 (259)	14.9	
	±9	±1		256 749.053 (246)	9.6	
	±7	±1		256 741.186 (243)	11.7	
	±10	±1		256 665.201 (254)	8.3	
	±8	±1		256 657.982 (245)	10.7	
	±11	±1		256 571.597 (267)	6.9	
	±9	±1		256 564.876 (251)	9.6	
	±12	±1		256 468.223 (286)	5.4	
	±10	±1		256 461.887 (261)	8.3	
	±13	±1		256 355.064 (311)	3.7	
	±11	±1		256 349.029 (276)	6.9	
	±14	±1		256 232.109 (341)	1.9	
	±12	±1		256 226.313 (297)	5.4	
	±13	±1		256 093.743 (324)	3.7	
	±14	±1		255 951.326 (356)	1.9	
16 - 15	±1	±1		274 459.400 (320)	15.9	
	±2	±1		274 219.421 (417)	15.8	
	±3	±1		274 186.961 (343)	15.4	
	0	±1		274 152.093 (392)	16.0	
	±1	±1		274 153.107 (332)	15.9	
	±4	±1		274 155.218 (323)	15.0	
	±2	±1		274 132.440 (319)	15.7	
	±5	±1		274 115.795 (313)	14.4	
	±3	±1		274 098.489 (314)	15.4	
	±6	±1		274 067.008 (307)	13.8	
	±4	±1		274 052.939 (309)	15.0	
	±7	±1		274 008.300 (302)	12.9	
	±5	±1		273 996.345 (306)	14.4	
	±8	±1		273 939.431 (300)	12.0	
	±6	±1		273 928.949 (303)	13.8	

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TABLE 7 : Microwave Spectrum of $\text{CH}_3\text{C} \equiv \text{CH}$ in the v_{10} Vibrational State (continued)

Transition J' J''	K	ℓ	Observed frequency (Estimated uncertainty)	Calculated frequency (Estimated uncertainty)	Line Strength	Reference
	±1	±1		273 922.595 (320)	15.9	
	±9	±1		273 860.281 (302)	10.9	
	±7	±1		273 850.870 (301)	12.9	
	±10	±1		273 770.780 (307)	9.7	
	±8	±1		273 762.178 (302)	12.0	
	±11	±1		273 670.891 (318)	8.4	
	±9	±1		273 662.909 (306)	10.9	
	±12	±1		273 560.588 (334)	7.0	
	±10	±1		273 553.091 (314)	9.7	
	±13	±1		273 439.855 (357)	5.4	
	±11	±1		273 432.740 (327)	8.4	
	±14	±1		273 308.678 (386)	3.8	
	±12	±1		273 301.868 (345)	7.0	
	±15	±1		273 167.050 (421)	1.9	
	±13	±1		273 160.483 (370)	5.4	
	±14	±1		273 008.591 (401)	3.8	
	±15	±1		273 846.197 (437)	1.9	
17 - 16	±1	±1		291 606.456 (390)	16.9	
	±2	±1		291 356.080 (506)	16.8	
	±3	±1		291 319.290 (419)	16.5	
	0	±1		291 275.340 (476)	17.0	
	±1	±1		291 278.718 (405)	16.9	
	±4	±1		291 284.796 (396)	16.1	
	±2	±1		291 257.527 (390)	16.8	
	±5	±1		291 242.526 (384)	15.5	
	±3	±1		291 221.838 (383)	16.5	
	±6	±1		291 190.460 (376)	14.9	
	±4	±1		291 173.670 (379)	16.1	
	±7	±1		291 127.930 (371)	14.1	
	±5	±1		291 113.692 (374)	15.5	
	±8	±1		291 054.646 (367)	13.2	
	±6	±1		291 042.194 (371)	14.9	
	±1	±1		291 036.101 (390)	16.9	
	±9	±1		290 970.466 (367)	12.2	
	±7	±1		290 959.318 (368)	14.1	
	±10	±1		290 875.308 (371)	11.1	
	±8	±1		290 865.146 (368)	13.2	
	±11	±1		290 769.126 (379)	9.9	
	±9	±1		290 759.724 (370)	12.2	
	±12	±1		290 651.986 (392)	8.5	
	±10	±1		290 643.084 (376)	11.1	
	±13	±1		290 523.571 (412)	7.1	
	±11	±1		290 515.247 (387)	9.9	
	±14	±1		290 384.167 (439)	5.4	
	±12	±1		290 376.224 (403)	8.5	
	±15	±1		290 233.662 (472)	3.8	
	±13	±1		290 226.028 (425)	7.1	
	±16	±1		290 072.051 (512)	1.9	
	±14	±1		290 064.664 (454)	5.4	
	±15	±1		290 892.141 (489)	3.8	
	±16	±1		289 708.460 (530)	1.9	

TABLE 8. Calculated Microwave Spectrum of $\text{CH}_3\text{C} \equiv \text{CH}$ in Order of Frequency.

Calculated frequency (Est. uncertainty) in MHz.	Vibr. State	Transition $J' - J''$	K	λ	Isotopic Species.	Calculated frequency (Est. uncertainty)	Vibr. State	Transition $J' - J''$	K	λ	Isotopic Species.
16 580.488 (6)		1 - 0	0	0	12 12 13	68 337.905 (20)		4 - 3	0	0	12 13 12
16 626.483 (8)		1 - 0	0	0	13 12 12	68 354.5029 (13)		4 - 3	\pm 3	0	
17 084.652 (7)		1 - 0	0	0	12 13 12	68 361.0359 (7)		4 - 3	\pm 2	0	
17 091.7425 (2)		1 - 0	0	0		68 364.9567 (7)		4 - 3	\pm 1	0	
17 139.623 (3)	v_{10}	1 - 0	0	\pm 1		68 366.2638 (7)		4 - 3	0	0	
33 160.288 (12)		2 - 1	\pm 1	0	12 12 13	68 492.040 (13)	v_{10}	4 - 3	\pm 1	\pm 1	
33 160.910 (12)		2 - 1	0	0	12 12 13	68 537.982 (10)	v_{10}	4 - 3	\pm 3	\mp 1	
33 252.277 (16)		2 - 1	\pm 1	0	13 12 12	68 547.127 (9)	v_{10}	4 - 3	\pm 2	\mp 1	
33 252.898 (16)		2 - 1	0	0	13 12 12	68 553.606 (9)	v_{10}	4 - 3	\pm 1	\mp 1	
34 168.583 (12)		2 - 1	\pm 1	0	12 13 12	68 554.194 (9)	v_{10}	4 - 3	\pm 3	\pm 1	
34 169.234 (12)		2 - 1	0	0	12 13 12	68 557.290 (9)	v_{10}	4 - 3	0	\pm 1	
34 182.7607 (4)		2 - 1	\pm 1	0		68 558.371 (9)	v_{10}	4 - 3	\pm 2	\pm 1	
34 183.4143 (5)		2 - 1	0	0		68 626.241 (13)	v_{10}	4 - 3	\pm 1	\pm 1	
34 246.305 (7)	v_{10}	2 - 1	\pm 1	\pm 1		82 807.110 (19)		5 - 4	\pm 3	0	12 12 13
34 277.186 (6)	v_{10}	2 - 1	\pm 1	\mp 1		82 894.881 (19)		5 - 4	\pm 2	0	12 12 13
34 279.126 (6)	v_{10}	2 - 1	0	\pm 1		82 899.545 (19)		5 - 4	\pm 1	0	12 12 13
34 313.405 (7)	v_{10}	2 - 1	\pm 1	\pm 1		82 901.100 (20)		5 - 4	0	0	12 12 13
49 737.465 (16)		3 - 2	\pm 2	0	12 12 13	83 117.110 (23)		5 - 4	\pm 3	0	13 12 12
49 740.263 (16)		3 - 2	\pm 1	0	12 12 13	83 124.865 (23)		5 - 4	\pm 2	0	13 12 12
49 741.197 (16)		3 - 2	0	0	12 12 13	83 129.519 (24)		5 - 4	\pm 1	0	13 12 12
49 875.455 (21)		3 - 2	\pm 2	0	13 12 12	83 131.070 (24)		5 - 4	0	0	13 12 12
49 878.248 (21)		3 - 2	\pm 1	0	13 12 12	85 407.204 (19)		5 - 4	\pm 3	0	12 13 12
49 879.179 (21)		3 - 2	0	0	13 12 12	85 415.340 (20)		5 - 4	\pm 2	0	12 13 12
51 249.768 (17)		3 - 2	\pm 2	0	12 13 12	85 420.224 (20)		5 - 4	\pm 1	0	12 13 12
51 252.698 (17)		3 - 2	\pm 1	0	12 13 12	85 421.852 (21)		5 - 4	0	0	12 13 12
51 253.675 (17)		3 - 2	0	0	12 13 12	85 442.6006 (14)		5 - 4	\pm 3	0	
51 271.0237 (6)		3 - 2	\pm 2	0		85 450.7660 (7)		5 - 4	\pm 2	0	
51 273.9646 (6)		3 - 2	\pm 1	0		85 455.6665 (6)		5 - 4	\pm 1	0	
51 274.9450 (6)		3 - 2	0	0		85 457.3002 (7)		5 - 4	0	0	
51 369.279 (10)	v_{10}	3 - 2	\pm 1	\pm 1		85 614.516 (14)	v_{10}	5 - 4	\pm 1	\pm 1	
51 410.651 (8)	v_{10}	3 - 2	\pm 2	\mp 1		85 671.852 (10)	v_{10}	5 - 4	\pm 3	\mp 1	
51 415.540 (8)	v_{10}	3 - 2	\pm 1	\mp 1		85 683.256 (9)	v_{10}	5 - 4	\pm 2	\mp 1	
51 418.388 (8)	v_{10}	3 - 2	0	\pm 1		85 691.289 (8)	v_{10}	5 - 4	\pm 1	\mp 1	
51 418.855 (8)	v_{10}	3 - 2	\pm 2	\pm 1		85 692.393 (9)	v_{10}	5 - 4	\pm 3	\pm 1	
51 469.930 (10)	v_{10}	3 - 2	\pm 1	\pm 1		85 695.709 (10)	v_{10}	5 - 4	0	\pm 1	
66 310.089 (18)		4 - 3	\pm 3	0	12 12 13	85 697.799 (10)	v_{10}	5 - 4	\pm 2	\pm 1	
66 316.307 (18)		4 - 3	\pm 2	0	12 12 13	85 782.268 (14)	v_{10}	5 - 4	\pm 1	\pm 1	
66 320.038 (19)		4 - 3	\pm 1	0	12 12 13	99 463.797 (17)		6 - 5	\pm 3	0	12 12 13
66 321.282 (19)		4 - 3	0	0	12 12 13	99 473.122 (17)		6 - 5	\pm 2	0	12 12 13
66 494.090 (24)		4 - 3	\pm 3	0	13 12 12	99 478.718 (18)		6 - 5	\pm 1	0	12 12 13
66 500.294 (24)		4 - 3	\pm 2	0	13 12 12	99 480.583 (19)		6 - 5	0	0	12 12 13
66 504.018 (24)		4 - 3	\pm 1	0	13 12 12	99 739.795 (20)		6 - 5	\pm 3	0	13 12 12
66 505.259 (24)		4 - 3	0	0	13 12 12	99 749.099 (20)		6 - 5	\pm 2	0	13 12 12
68 326.185 (19)		4 - 3	\pm 3	0	12 13 12	99 754.683 (21)		6 - 5	\pm 1	0	13 12 12
68 332.695 (19)		4 - 3	\pm 2	0	12 13 12	99 756.545 (22)		6 - 5	0	0	13 12 12
68 336.602 (20)		4 - 3	\pm 1	0	12 13 12	102 487.371 (18)		6 - 5	\pm 3	0	12 13 12

TABLE 8 : Calculated Microwave Spectrum of $\text{CH}_3\text{C} \equiv \text{CH}$ in order of Frequency. (continued)

Calculated frequency (Est. uncertainty) in MHz.	Vibr. State	Transition $J' - J''$	K	λ	Isotopic Species.	Calculated frequency (Est. uncertainty) in MHz.	Vibr. State	Transition $J' - J''$	K	λ	Isotopic Species.
102 497.634 (18)		6 - 5	\pm 2	0	12 13 12	136 704.5011 (13)		8 - 7	\pm 3	0	
102 503.492 (19)		6 - 5	\pm 1	0	12 13 12	136 717.5599 (6)		8 - 7	\pm 2	0	
102 505.446 (20)		6 - 5	0	0	12 13 12	136 725.3972 (4)		8 - 7	\pm 1	0	
102 530.3464 (14)		6 - 5	\pm 3	0		136 728.0100 (5)		8 - 7	0	0	
102 540.1437 (7)		6 - 5	\pm 2	0		136 979.524 (30)	v_{10}	8 - 7	\pm 1	\pm 1	
102 546.0235 (5)		6 - 5	\pm 1	0		137 070.621 (22)	v_{10}	8 - 7	\pm 3	\mp 1	
102 547.9837 (6)		6 - 5	0	0		137 088.647 (23)	v_{10}	8 - 7	\pm 2	\mp 1	
102 736.636 (16)	v_{10}	6 - 5	\pm 1	\pm 1		137 101.080 (25)	v_{10}	8 - 7	\pm 1	\mp 1	
102 805.304 (9)	v_{10}	6 - 5	\pm 3	\mp 1		137 105.406 (25)	v_{10}	8 - 7	\pm 3	\pm 1	
102 818.937 (8)	v_{10}	6 - 5	\pm 2	\mp 1		137 106.873 (37)	v_{10}	8 - 7	0	\pm 1	
102 828.492 (9)	v_{10}	6 - 5	\pm 1	\mp 1		137 115.336 (39)	v_{10}	8 - 7	\pm 2	\pm 1	
102 830.359 (9)	v_{10}	6 - 5	\pm 3	\pm 1		137 247.926 (30)	v_{10}	8 - 7	\pm 1	\pm 1	
102 833.526 (14)	v_{10}	6 - 5	0	\pm 1		149 191.204 (17)		9 - 8	\pm 3	0	12 12 13
102 837.117 (15)	v_{10}	6 - 5	\pm 2	\pm 1		149 205.184 (19)		9 - 8	\pm 2	0	12 12 13
102 937.938 (16)	v_{10}	6 - 5	\pm 1	\pm 1		149 213.574 (21)		9 - 8	\pm 1	0	12 12 13
116 040.086 (14)		7 - 6	\pm 3	0	12 12 13	149 216.372 (22)		9 - 8	0	0	12 12 13
116 050.962 (15)		7 - 6	\pm 2	0	12 12 13	149 605.162 (23)		9 - 8	\pm 3	0	13 12 12
116 057.490 (17)		7 - 6	\pm 1	0	12 12 13	149 619.112 (24)		9 - 8	\pm 2	0	13 12 12
116 059.667 (18)		7 - 6	0	0	12 12 13	149 627.484 (26)		9 - 8	\pm 1	0	13 12 12
119 362.077 (15)		7 - 6	\pm 3	0	13 12 12	149 630.275 (27)		9 - 8	0	0	13 12 12
119 372.930 (16)		7 - 6	\pm 2	0	13 12 12	153 727.055 (16)		9 - 8	\pm 3	0	12 13 12
119 379.444 (18)		7 - 6	\pm 1	0	13 12 12	153 741.688 (19)		9 - 8	\pm 2	0	12 13 12
119 381.616 (19)		7 - 6	0	0	13 12 12	153 750.470 (21)		9 - 8	\pm 1	0	12 13 12
119 568.116 (15)		7 - 6	\pm 3	0	12 13 12	153 753.398 (21)		9 - 8	0	0	12 13 12
119 579.503 (16)		7 - 6	\pm 2	0	12 13 12	153 790.7695 (15)		9 - 8	\pm 3	0	
119 586.337 (18)		7 - 6	\pm 1	0	12 13 12	153 805.4578 (8)		9 - 8	\pm 2	0	
119 588.615 (19)		7 - 6	0	0	12 13 12	153 814.2731 (6)		9 - 8	\pm 1	0	
119 617.6700 (14)		7 - 6	\pm 3	0		153 817.2119 (6)		9 - 8	0	0	
119 629.0984 (6)		7 - 6	\pm 2	0		154 100.149 (44)	v_{10}	9 - 8	\pm 1	\pm 1	
119 635.9573 (4)		7 - 6	\pm 1	0		154 202.319 (37)	v_{10}	9 - 8	\pm 3	\mp 1	
119 638.2438 (5)		7 - 6	0	0		154 222.493 (38)	v_{10}	9 - 8	\pm 2	\mp 1	
119 858.329 (21)	v_{10}	7 - 6	\pm 1	\pm 1		154 236.272 (42)	v_{10}	9 - 8	\pm 1	\mp 1	
119 938.255 (13)	v_{10}	7 - 6	\pm 3	\mp 1		154 242.161 (56)	v_{10}	9 - 8	0	\pm 1	
119 954.099 (12)	v_{10}	7 - 6	\pm 2	\mp 1		154 242.394 (42)	v_{10}	9 - 8	\pm 3	\pm 1	
119 965.121 (14)	v_{10}	7 - 6	\pm 1	\mp 1		154 254.193 (60)	v_{10}	9 - 8	\pm 2	\pm 1	
119 968.046 (14)	v_{10}	7 - 6	\pm 3	\pm 1		154 402.102 (44)	v_{10}	9 - 8	\pm 1	\pm 1	
119 970.621 (23)	v_{10}	7 - 6	0	\pm 1		165 765.905 (22)		10 - 9	\pm 3	0	12 12 13
119 976.304 (24)	v_{10}	7 - 6	\pm 2	\pm 1		165 781.436 (24)		10 - 9	\pm 2	0	12 12 13
120 093.181 (21)	v_{10}	7 - 6	\pm 1	\pm 1		165 790.757 (26)		10 - 9	\pm 1	0	12 12 13
132 615.909 (14)		8 - 7	\pm 3	0	12 12 13	165 793.864 (27)		10 - 9	0	0	12 12 13
132 626.338 (16)		8 - 7	\pm 2	0	12 12 13	166 225.030 (33)		10 - 9	\pm 3	0	13 12 12
132 635.798 (18)		8 - 7	\pm 1	0	12 12 13	166 241.327 (34)		10 - 9	\pm 2	0	13 12 12
132 638.284 (19)		8 - 7	0	0	12 12 13	166 250.627 (36)		10 - 9	\pm 1	0	13 12 12
132 983.889 (15)		8 - 7	\pm 3	0	13 12 12	166 253.728 (37)		10 - 9	0	0	13 12 12
132 996.291 (17)		8 - 7	\pm 2	0	13 12 12	170 805.606 (20)		10 - 9	\pm 3	0	12 13 12
133 003.734 (19)		8 - 7	\pm 1	0	13 12 12	170 821.860 (22)		10 - 9	\pm 2	0	12 13 12
133 006.215 (20)		8 - 7	0	0	13 12 12	170 831.615 (24)		10 - 9	\pm 1	0	12 13 12
136 647.868 (14)		8 - 7	\pm 3	0	12 13 12	170 834.867 (25)		10 - 9	0	0	12 13 12
136 660.879 (16)		8 - 7	\pm 2	0	12 13 12	170 876.4050 (20)		10 - 9	\pm 3	0	
136 668.687 (18)		8 - 7	\pm 1	0	12 13 12	170 892.7218 (11)		10 - 9	\pm 2	0	
136 671.290 (19)		8 - 7	0	0	12 13 12	170 902.5144 (9)		10 - 9	\pm 1	0	

TABLE 8 : Calculated Microwave Spectrum of $\text{CH}_3\text{C} \equiv \text{CH}$ in order of Frequency. (continued)

Calculated frequency (Est. uncertainty) in MHz.	Vibr. State	Transition $J' - J''$	K	ℓ	Isotopic Species.	Calculated frequency (Est. uncertainty) in Mhz.	Vibr. State	Transition $J' - J''$	K	ℓ	Isotopic Species.
170 905 7790 (9)		10 - 9	0			205 636.291 (124)	v_{10}	12 - 11	± 1	∓ 1	
171 220.133 (64)	v_{10}	10 - 9	± 1	± 1		205 641.043 (153)	v_{10}	12 - 11	0	± 1	
171 333.266 (57)	v_{10}	10 - 9	± 3	∓ 1		205 650.656 (128)	v_{10}	12 - 11	± 3	± 1	
171 355.552 (59)	v_{10}	10 - 9	± 2	∓ 1		205 669.488 (163)	v_{10}	12 - 11	± 2	± 1	
171 370.601 (63)	v_{10}	10 - 9	± 1	∓ 1		205 860.498 (122)	v_{10}	12 - 11	± 1	± 1	
171 376.366 (82)	v_{10}	10 - 9	0	± 1		215 485.824 (19)		13 - 12	± 3	0	12 12 13
171 378.963 (65)	v_{10}	10 - 9	± 3	± 1		215 505.999 (21)		13 - 12	± 2	0	12 12 13
171 392.852 (87)	v_{10}	10 - 9	± 2	± 1		215 518.108 (24)		13 - 12	± 1	0	12 12 13
171 555.636 (64)	v_{10}	10 - 9	± 1	± 1		215 522.145 (23)		13 - 12	0	0	12 12 13
182 339.951 (26)		11 - 10	± 3	0	12 12 13	216 083.511 (34)		13 - 12	± 3	0	13 12 12
182 357.031 (27)		11 - 10	± 2	0	12 12 13	216 103.641 (35)		13 - 12	± 2	0	13 12 12
182 367.281 (29)		11 - 10	± 1	0	12 12 13	216 115.723 (38)		13 - 12	± 1	0	13 12 12
182 370.699 (30)		11 - 10	0	0	12 12 13	216 119.751 (39)		13 - 12	0	0	13 12 12
182 845.823 (40)		11 - 10	± 3	0	13 12 12	222 036.723 (20)		13 - 12	± 3	0	12 13 12
182 862.865 (42)		11 - 10	± 2	0	13 12 12	222 057.832 (23)		13 - 12	± 2	0	12 13 12
182 873.094 (43)		11 - 10	± 1	0	13 12 12	222 070.500 (25)		13 - 12	± 1	0	12 13 12
182 876.503 (44)		11 - 10	0	0	13 12 12	222 074.723 (26)		13 - 12	0	0	12 13 12
187 883.449 (21)		11 - 10	± 3	0	12 13 12	222 128.8138 (63)		13 - 12	± 3	0	
187 901.323 (23)		11 - 10	± 2	0	12 13 12	222 150.0089 (33)		13 - 12	± 2	0	
187 912.050 (25)		11 - 10	± 1	0	12 13 12	222 162.7292 (22)		13 - 12	± 1	0	
187 915.626 (26)		11 - 10	0	0	12 13 12	222 166.9698 (23)		13 - 12	0	0	
187 961.3376 (29)		11 - 10	± 3	0		222 575.529 (160)	v_{10}	13 - 12	± 1	± 1	
187 979.2818 (16)		11 - 10	± 2	0		222 720.762 (154)	v_{10}	13 - 12	± 3	∓ 1	
187 990.0510 (12)		11 - 10	± 1	0		222 749.121 (157)	v_{10}	13 - 12	± 2	∓ 1	
187 993.6412 (13)		11 - 10	0	0		222 767.459 (165)	v_{10}	13 - 12	± 1	∓ 1	
188 339.405 (90)	v_{10}	11 - 10	± 1	± 1		222 771.274 (200)	v_{10}	13 - 12	0	± 1	
188 463.378 (83)	v_{10}	11 - 10	± 3	∓ 1		222 785.687 (170)	v_{10}	13 - 12	± 3	± 1	
188 487.735 (86)	v_{10}	11 - 10	± 2	∓ 1		222 807.422 (213)	v_{10}	13 - 12	± 2	± 1	
188 503.973 (91)	v_{10}	11 - 10	± 1	∓ 1		223 011.683 (160)	v_{10}	13 - 12	± 1	± 1	
188 509.367 (114)	v_{10}	11 - 10	0	± 1		223 057.529 (24)		14 - 13	± 3	0	12 12 13
188 515.065 (93)	v_{10}	11 - 10	± 3	± 1		232 079.251 (27)		14 - 13	± 2	0	12 12 13
188 531.291 (121)	v_{10}	11 - 10	± 2	± 1		232 092.288 (30)		14 - 13	± 1	0	12 12 13
188 708.459 (90)	v_{10}	11 - 10	± 1	± 1		232 096.634 (32)		14 - 13	0	0	12 12 13
198 913.277 (25)		12 - 11	± 3	0	12 12 13	232 701.067 (27)		14 - 13	± 3	0	13 12 12
198 931.906 (27)		12 - 11	± 2	0	12 12 13	232 722.740 (32)		14 - 13	± 2	0	13 12 12
198 943.086 (24)		12 - 11	± 1	0	12 12 13	232 735.747 (37)		14 - 13	± 1	0	13 12 12
198 946.813 (30)		12 - 11	0	0	12 12 13	232 740.083 (39)		14 - 13	0	0	13 12 12
199 465.073 (42)		12 - 11	± 3	0	13 12 12	239 112.009 (46)		14 - 13	± 3	0	12 13 12
199 483.660 (43)		12 - 11	± 2	0	13 12 12	239 134.732 (47)		14 - 13	± 2	0	12 13 12
199 494.815 (45)		12 - 11	± 1	0	13 12 12	239 148.369 (50)		14 - 13	± 1	0	12 13 12
199 498.534 (45)		12 - 11	0	0	13 12 12	239 152.915 (50)		14 - 13	0	0	12 13 12
204 960.512 (19)		12 - 11	± 3	0	12 13 12	239 211.2176 (89)		14 - 13	± 3	0	
204 980.004 (21)		12 - 11	± 2	0	12 13 12	239 234.0360 (50)		14 - 13	± 2	0	
204 991.703 (24)		12 - 11	± 1	0	12 13 12	239 247.7306 (35)		14 - 13	± 1	0	
204 995.603 (25)		12 - 11	0	0	12 13 12	239 252.2960 (35)		14 - 13	0	0	
205 045.4972 (43)		12 - 11	± 3	0		239 692.238 (206)	v_{10}	14 - 13	± 1	± 1	
205 065.0675 (22)		12 - 11	± 2	0		239 847.868 (199)	v_{10}	14 - 13	± 3	∓ 1	
205 076.8127 (16)		12 - 11	± 1	0		239 878.150 (203)	v_{10}	14 - 13	± 2	∓ 1	
205 080.7282 (16)		12 - 11	0	0		239 897.382 (212)	v_{10}	14 - 13	± 1	∓ 1	
205 457.894 (122)	v_{10}	12 - 11	± 1	± 1		239 899.939 (255)	v_{10}	14 - 13	0	± 1	
205 592.571 (115)	v_{10}	12 - 11	± 3	∓ 1		239 920.113 (219)	v_{10}	14 - 13	± 3	± 1	
205 618.952 (118)	v_{10}	12 - 11	± 2	∓ 1		239 945.070 (271)	v_{10}	14 - 13	± 2	± 1	

TABLE 8 : Calculated Microwave Spectrum of $\text{CH}_3\text{C} \equiv \text{CH}$ in Order of Frequency. (continued)

Calculated frequency (Est. uncertainty) in MHz.	Vibr. State	Transition $J' - J''$	K	ℓ	Isotopic Species.	Calculated frequency (Est. uncertainty) in MHz.	Vibr. State	Transition $J' - J''$	K	ℓ	Isotopic Species
240 161.943 (206)	v_{10}	14 - 13	± 1	± 1		281 814.455 (234)		17 - 16	0	0	12 12 13
248 628.335 (61)		15 - 14	± 3	0	12 12 13	282 547.746 (284)		17 - 16	± 3	0	13 12 12
248 651.602 (64)		15 - 14	± 2	0	12 12 13	282 574.037 (289)		17 - 16	± 2	0	13 12 12
248 665.566 (67)		15 - 14	± 1	0	12 12 13	282 589.815 (294)		17 - 16	± 1	0	13 12 12
248 670.221 (68)		15 - 14	0	0	12 12 13	282 595.075 (295)		17 - 16	0	0	13 12 12
249 317.672 (68)		15 - 14	± 3	0	13 12 12	290 331.578 (299)		17 - 16	± 3	0	12 13 12
249 340.885 (73)		15 - 14	± 2	0	13 12 12	290 359.131 (301)		17 - 16	± 2	0	12 13 12
249 354.817 (77)		15 - 14	± 1	0	13 12 12	290 381.180 (305)		17 - 16	0	0	12 13 12
249 359.462 (79)		15 - 14	0	0	13 12 12	290 452.2550 (237)		17 - 16	± 3	0	
256 186.296 (98)		15 - 14	± 3	0	12 13 12	290 479.9335 (168)		17 - 16	± 2	0	
256 210.631 (100)		15 - 14	± 2	0	12 13 12	290 496.5449 (143)		17 - 16	± 1	0	
256 225.236 (101)		15 - 14	± 1	0	12 13 12	290 502.0827 (140)		17 - 16	0	0	
256 230.105 (102)		15 - 14	0	0	12 13 12	291 036.101 (390)	v_{10}	17 - 16	± 1	± 1	
256 292.6389 (125)		15 - 14	± 3	0		291 221.838 (383)	v_{10}	17 - 16	± 3	∓ 1	
256 317.0790 (76)		15 - 14	± 2	0		291 257.527 (390)	v_{10}	17 - 16	± 2	∓ 1	
256 331.7469 (58)		15 - 14	± 1	0		291 275.340 (476)	v_{10}	17 - 16	0	± 1	
256 336.6368 (57)		15 - 14	0	0		291 278.718 (405)	v_{10}	17 - 16	± 1	∓ 1	
256 807.951 (259)	v_{10}	15 - 14	± 1	± 1		291 319.290 (419)	v_{10}	17 - 16	± 3	± 1	
256 973.805 (252)	v_{10}	15 - 14	∓ 3	∓ 1		291 356.080 (506)	v_{10}	17 - 16	± 2	± 1	
257 005.951 (257)	v_{10}	15 - 14	± 2	∓ 1		291 606.456 (390)	v_{10}	17 - 16	± 1	± 1	
257 025.963 (268)	v_{10}	15 - 14	± 1	∓ 1							
257 026.919 (319)	v_{10}	15 - 14	0	± 1							
257 053.886 (277)	v_{10}	15 - 14	± 3	± 1							
257 082.410 (339)	v_{10}	15 - 14	± 2	± 1							
257 311.205 (259)	v_{10}	15 - 14	± 1	± 1							
265 198.183 (127)		16 - 15	± 3	0	12 12 13						
265 222.993 (131)		16 - 15	± 2	0	12 12 13						
265 237.883 (133)		16 - 15	± 1	0	12 12 13						
265 242.847 (135)		16 - 15	0	0	12 12 13						
265 933.255 (154)		16 - 15	± 3	0	13 12 12						
265 958.008 (158)		16 - 15	± 2	0	13 12 12						
265 972.864 (162)		16 - 15	± 1	0	13 12 12						
265 977.816 (164)		16 - 15	0	0	13 12 12						
273 259.510 (180)		16 - 15	± 3	0	12 13 12						
273 285.456 (182)		16 - 15	± 2	0	12 13 12						
273 301.027 (184)		16 - 15	± 1	0	12 13 12						
273 306.218 (185)		16 - 15	0	0	12 13 12						
273 373.0079 (174)		16 - 15	± 3	0							
273 399.0681 (114)		16 - 15	± 2	0							
273 414.7083 (93)		16 - 15	± 1	0							
273 419.9223 (91)		16 - 15	0	0							
273 922.595 (320)	v_{10}	16 - 15	± 1	± 1							
274 098.489 (314)	v_{10}	16 - 15	± 3	∓ 1							
274 132.440 (319)	v_{10}	16 - 15	± 2	∓ 1							
274 152.093 (392)	v_{10}	16 - 15	0	± 1							
274 153.107 (332)	v_{10}	16 - 15	± 1	∓ 1							
274 186.961 (343)	v_{10}	16 - 15	± 3	± 1							
274 219.421 (417)	v_{10}	16 - 15	± 2	± 1							
274 459.400 (320)	v_{10}	16 - 15	± 1	± 1							
281 767.016 (225)		17 - 16	± 3	0	12 12 13						
281 793.367 (229)		17 - 16	± 2	0	12 12 13						
281 809.183 (233)		17 - 16	± 1	0	12 12 13						

3.1. CH₃CCH References

a. Primary References

- [50A] Ralph Trambarulo and Walter Gordy, J. Chem. Phys. **18**, 1613 (1950). "The Microwave Spectrum and Structure of Methyl acetylene".
- [57A] C. A. Burrus and Walter Gordy, J. Chem. Phys. **26**, 391 (1957). "Spectra of some Symmetric Top Molecules in the one-to-four Millimeter Wave Region".
- [66A] J. S. Muenter and V. W. Laurie, J. Chem. Phys. **45**, 885 (1966). "Deuterium Isotope Effects on Molecular Dipole Moments by Microwave Spectroscopy".
- [69A] Agnès Bauer and Jean Burie, Compt. Rend. Acad. Sci. **268 B**, 800 (1969). "Spectre de rotation du propyne en ondes millimétriques".
- [69B] R. L. Shoemaker and W. H. Flygare, J. Am. Chem. Soc. **91**, 5417 (1969). "Magnetic susceptibility Anisotropy, Molecular Quadrupole Moment, Molecular *g* values, and the Sign of the Electric Dipole Moment in Methylacetylene".
- [73A] J. L. Duncan, D. C. Mc Kean, P. D. Mallinson, and R. D. Mc Culloch, J. Mol. Spectrosc. **46**, 232 (1973). "Infrared Spectra of CHD₂Cl and CHD₂CCH and the Geometries of Methyl Chloride and Propyne".
- [75A] L. Engelbrecht and D. H. Sutter, Z. Naturforsch. **30a**, 1265 (1976). "Comment on the Analysis of Microwave Rotational Zeeman Effect Spectra of Symmetric Top Molecules".
- [76A] J. L. Duncan, J. Mol. Spectrosc. **60**, 225 (1976). "The centrifugal Distortion Constant *D_K* of Symmetric Top Molecules".
- [78A] A. Dubrule, D. Boucher, J. Burie, and J. Demaison, J. Mol. Spectrosc. **72**, 158 (1978). "Microwave Spectra of Propyne and its [13C] Isotopic Species. Refined Molecular Structure of Propyne".
- J. T. Cox, P. B. Peyton, and Walter Gordy, Phys. Rev. **91**, 222 (1953). "Zeeman Effect in the Microwave Spectra of Methyl Fluoride and Methyl Acetylene".
- L. F. Thomas, E. I. Sherrard, and John Sheridan, Trans. Farad. Soc. **51**, 619 (1955). "Microwave Spectra of some partially Deuteriated Methyl Derivatives I. Methyl Cyanide and Methyl Acetylene".
- T. S. Jaseja, Proc. Indian Acad. Sci. **50A**, 108 (1959). "The Microwave Spectrum of Methyl Cyanide and l-type Doubling in CH₃CN, CH₃NC, CH₃CCH, and CF₃CCH".
- C. C. Costain, J. Chem. Phys. **29**, 864 (1958). "Determination of Molecular Structures from Ground State Rotational Constants".
- J. T. Cox and Walter Gordy, Phys. Rev. **101**, 1298 (1956). "Zeeman Effect of some Linear and Symmetric Top Molecules".
- G. G. Weber, J. Mol. Spectrosc. **10**, 321 (1963). "On the l-type Doubling and l-type Resonance of Molecules in the Microwave Region".
- V. W. Weiss and W. H. Flygare, J. Chem. Phys. **45**, 8 (1966). "Deuterium Nuclear Quadrupole Interaction in FC≡CD, CH₃C≡CD, and ClC≡CD".
- A. J. Roberts, T. K. Tung and C. C. Lin, J. Chem. Phys. **48**, 4046 (1968). "Linewidths of the Rotational Spectra of Symmetric Top Molecules".
- L. H. Sharpen, J. S. Muenter and V. W. Laurie, J. Chem. Phys. **53**, 2513 (1970). "Electric Polarizability Anisotropies of Nitrous Oxide, Propyne, and Carbonyl Sulfide by Microwave Spectroscopy".
- S. C. M. Luijendijk, J. Phys. B. **10**, 1735 (1977). "On the Shape of Pressure-broadened Absorption lines in the Microwave Region I. Deviations from the Lorentzian line Shape".
- S. C. M. Luijendijk, J. Phys. B. **10**, 1741 (1977). "On the Shape of Pressure broadened Absorption Lines in the Microwave Region II. Collision-induced width and Shift of some Rotational Absorption Lines as a Function of Temperature".

b. Other References

- C. M. Johnson, Ralph Trambarulo, and Walter Gordy, Phys. Rev. **84**, 1178 (1951). "Microwave Spectroscopy in the region from two to three Millimeters".
- S. N. Ghosh, Ralph Trambarulo, and Walter Gordy, Phys. Rev. **87**, 172 (1952). "Dipole Moments of Several Molecules from Their Microwave Spectra".
- S. N. Ghosh, Ralph Trambarulo, and Walter Gordy, J. Chem. Phys. **21**, 308 (1953). "Electric Dipole Moments of Several Molecules from the Stark Effect".

c. Interstellar References

- L. E. Snyder and D. Buhl, Nature (Phys. Sci.) **243**, 45 (1973). "Interstellar Methylacetylene and Isocyanic Acid".
- W. F. Huebner, D. Buhl, and L. E. Snyder, Astronom. J. **81**, 671 (1976). "Microwave Line Transitions in the 3-mm wavelength Range in Comet Kohoutek (1973 f)".
- F. J. Lovas, D. R. Johnson, D. Buhl and L. E. Snyder, Astrophys. J. **209**, 770 (1976). "Millimeter Emission Lines in Orion A".