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Microwave Rotational Components of the $\nu_9 = 1$ and $\nu_{10} = 2$ Vibrational Modes of $^{13}CH_3CCH$ Molecule In the Range 16 – 50 GHz

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Abstract

Some rotational components have been measured in the ground, the $\nu_9 = 1$ and the $\nu_{10} = 2$ vibrational states for $^{13}CH_3CCH$ isotopic species in the frequency range 16–50 GHz. A set of rotational constants has been determined, which gives the best fit between the observed and the calculated frequencies, for each vibrational state. A Fermi resonance was found between these two states.

Key Words: Microwave spectra; Rotational spectra; Propyne; Interstellar clouds; Fermi resonance; Vibrational modes.

1. Introduction

Propyne (CH_3CCH) is an abundant species in interstellar clouds [1]. Its infrared spectrum has been observed in the atmosphere of Titan, Jupiter and the seventh moon of Saturn [2], while its microwave spectrum has been detected in the Taurus dark clouds [3] and in Orion A [4]. Although propyne and its isotopic species have been studied in the microwave region [5–11] and in the infrared region [12–24], many features of its spectra are still to be explained, especially the different interactions between some of its vibrational levels. This is not strange for this molecule with small dipole moment (0.7829D) [15]. The molecule (see Figure 1) has ten vibrational modes which fall into two classes: 5 single vibrations in the A_1 class, which will give rise to parallel type bands; and 5 two-fold degenerate vibrations in the E class which produce perpendicular type bands (see Table 1). Since its dipole moment is small, a thermal population distribution exists in most of its low-lying excited vibrational states. Thus propyne is well-suited to help determine the kinetic temperature of interstellar clouds.

The goal of this work is the measurement of some rotational components in the $\nu_9 = 1$ and $\nu_{10} = 2$ vibrational states of the $^{13}CH_3CCH$ isotopomer, to determine a more accurate set of rotational constants for ^{13}C tagged species, measurements which are useful to more accurately determine the structure of propyne. Also we attain a better understanding of the interactions between the $\nu_9 = 1$ and the $\nu_{10} = 2$ vibrational states by utilizing the method of select isotopic substitution to bring these levels closer wherein the interaction becomes stranger.

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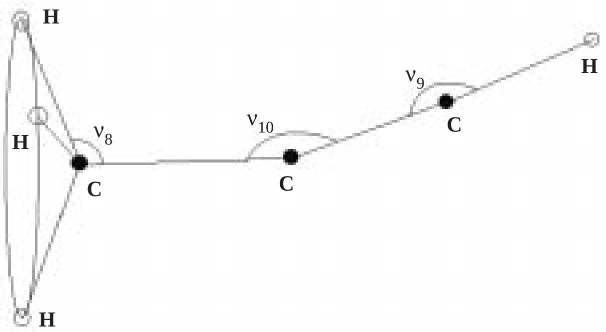

Figure 1. Schematic diagram of the CH_3CCH molecule with the ν_8, ν_9 and ν_{10} vibrational modes.

Table 1. The frequency of the ten vibrational state of the CH_3CCH and $^{13}CH_3CCH$ isotopomers.

mode	Discription of the mode	Symmetry	CH_3CCH (cm^{-1})	$^{13}CH_3CCH$ (cm^{-1})*	Reference**
ν_1	Acetylenic C-H stretching	A_1	3335.1	3335.1	22
ν_2	Methyl group H-C symmetric stretching	A_1	2910	2906.1	22
ν_3	C≡C stretching	A_1	2137.88	2136.51	14
ν_4	CH_3 deformation	A_1	1385.588	1375.59	23
ν_5	C-C stretching	A_1	930.276577	913.80	29
ν_6	Methyl group H-C antisymmetric stretching	E	2980.8	2971.1	22
ν_7	Degenerate CH_3 deformation	E	1450.28	1448.73	23
ν_8	CH_3rocking	E	1036.147557	1027.94	29
ν_9	C≡C-H bending	E	638.57068	638.56	17
ν_{10}	C-C≡C bending	E	330.93811	330.64	16
$\nu_{10} = 2$	First overtone of ν_{10}	E	662.0•	652.7	15

*Calculated by subtracting the frequency shift due to ^{13}C substitution that given by Duncan et al [25] from the values for CH_3CCH.

**This reference for the value of the vibrational frequency of the mode for CH_3CCH.

• This value is the band origin (Ref [15]), while Ref. [18] reported the values of the two contours $\nu_{10} = 2$, $\ell = 0$ and $\nu_{10} = 2, \ell = \pm 2$ to be 650.86207 cm^{-1} and 671.31006 cm^{-1}, respectively.

The molecular spectra and structure of ^{13}C tagged isotopomers of propyne were originally studied by Trambarulo and Gordy [5], investigating the microwave spectra in the ground vibrational state of six isotopomers of propyne: one of which is $^{13}CH_3CCH$. Dubrulle et al. [6] have studied the microwave spectra of the ground vibrational state of propyne and its ^{13}C isotopic species with molecular beam spectroscopy. Bauer et al. [7] and Tam et al. [11] have studied the microwave spectra of ^{13}C substituted propyne in the ground and ν_{10} =1 vibrational states. Duncan et al. [25] have studied the harmonic force field of propyne ^{13}C tagged isotopomers and reported the effect of the ^{13}C substitution on the frequencies of the ten vibrational states , but these studies have not fully determined its molecular structure. Le Guennec et al. [2] have measured some rotational components in the ground vibrational state for ^{13}C tagged isotopomers CH_2DCCH and CH_3CCD.

2. Experimental Details

The microwave measurements reported in this work were made using the microwave spectrometer (see Figure 2) that was desribed earlier [9]. For convenience, we describe it briefly here. It consists of three parts: the first part is the radiation source, where two Klystrons; the first is an OKI 14V10, and the second an is OKI 24V10, which consisted of giving fundamental frequencies in the range 12–16 GHz, and 22–26 GHz, respectively. A crossed wave guide multiplier [26] was used to provide radiation in the 33 GHz and the 49 GHz regions via the second harmonic of both Klystrons, respectively. The second part is the absorption cell which was made from soft drawn copper refrigeration tubing of length 66 m and diameter 16 mm. The absorption cell was evacuated using an oil vapor diffusion pump cold-tapped with liquid nitrogen and was continuously pumped by a mechanical pump. The third part is for detection and display of the signal. The microwave signals were detected using a variety of crystal diodes and the spectral lines were displayed on a dual pen chart recorder with the upper pen recording the frequency markers and the other pen recording the spectral profiles (see Figure 3).

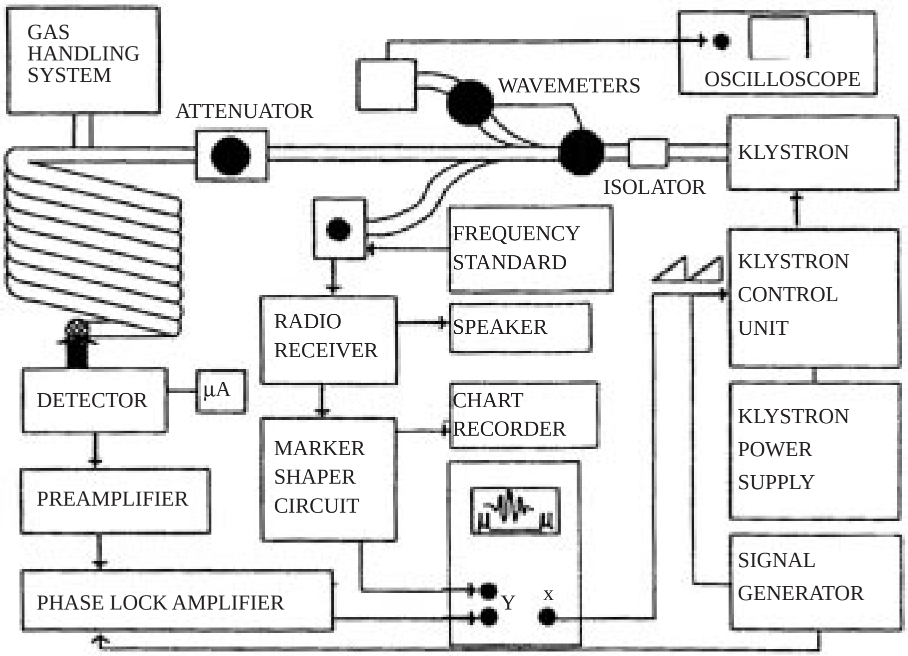

Figure 2. A block diagram of the spectrometer used to make the measurements in this work.

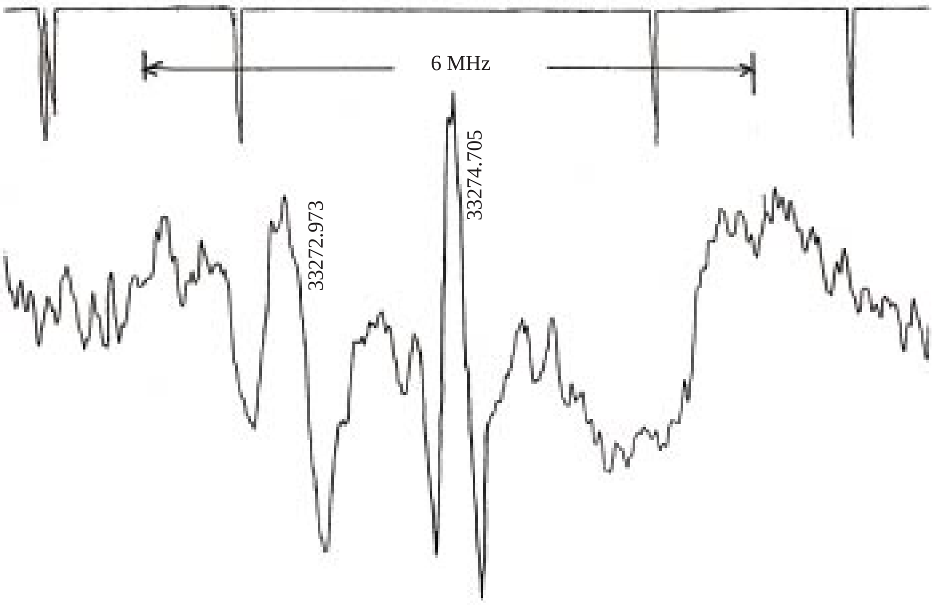

Figure 3. Dual pen chart recorder scan of some rotational components of $\Delta J = 2 \leftarrow 1$ of the $\nu_9 = 1$. The lower pen records the absorption profile, while the upper one records the markers.

The use of chart recording allows long-term scanning over only a few megahertz. A typical scan rate may be 3 MHz over a time interval of 3–5 minutes. This allows good signal integration and noise filtering over the interval. The frequency interval is scaled by using a set of markers generated as a beat note between the standard frequency source and the Klystron frequency, as the Klystron is swept over its frequeny range. These markers serve to partition the frequency profile interval and establish the absolute value of each frequency line. Once ten or more scans have been acquired for each line with overall repeatability less than 300 KHz, the spectral line is assumed to be satisfactorily measured and the results are tabulated.

Commercial samples of ^{13}CH$_3$CCH of 98.55% concentration ^{13}C were obtained from Merck Frosst Canada Inc. [27]. In preparation for the system to receive each sample, the cold trap was frozen under vacuum conditions and any extra gases were pumped away using a cold-trapped diffusion pump vacuum system in the standard way. Calibrated samples of 1–2 mTorr of vapor were admitted into the vacuum chamber as wanted, each time a measurement was made.

3. Theoretical Formula

A theoretical model was used in this work for the calculations of frequencies of rotational transitions $(J+1) \leftarrow J$ and was derived by Rhee and Roberts [10] and was put in a new form by Gadhi et al. [1], while the symbols have their usual meaning as given in reference [10]. For convenience, some of them will be given here, B_{v} and A_{v} are the principal rotational constants, $X_{\ell\ell}$ is the anharmonic constant, ζ is the coriolis coupling constant, D_J, D_{JK} and D_K are the first order centrifugal distortion constants, $\gamma_{\ell\ell} = B_3$ is the coriolis centrifugal distortion constant, η_{J}, η_{JJ} and η_{JK} are the higher order diagonal matrix elements. This representaion has an advantage in that it can be used to calculate rotational frequencies for any vibrational state with no need to have different vibrational levels (Eq. 1).

$$
\begin{aligned}
\upsilon(V,J,K,\ell) \quad = \quad & 2(J+1)\{[B_v + \gamma_{\ell\ell}\ell^2 - D_{Jk}k^2 - 2D_J(J+1)^2] \\
& +[\eta_{\mathrm{J}}K\ell + \eta_{\mathrm{Jk}}K^3\ell + 2\eta_{\mathrm{JJ}}K\ell(J+1)^2] \\
& \mp[q_v(v+1)_{k\ell=\mp1} + f_{24}v(v+2)_{\substack{K=\pm1 \\ \ell=\mp2}}]\} \qquad (1) \\
& \pm[(b^{2\pm}_{1,v,\ell}/C^{\pm}_{1})_{K\ell\neq1}q_v^2 + (b^{2\mp}_{2,v,\ell}/C^{\pm}_{2})_{K\ell\neq-2}f_{24}^2] \\
& [a^{2\pm}_{2,J+1,K} - a^{2\pm}_{2,J,K}] \pm [(b^{2\pm}_{1,v,\ell})/C^{\mp}_{3}] \\
& [a^{2\pm}_{1,J+1,K} - a^{2\pm}_{1,J,K}][q_{12}(2K\pm1) + d_{12}(\ell\mp1)]^2,
\end{aligned}
$$

where:

$$
\begin{aligned}
& a^{2\pm}_{n,J,K} = \prod_{n=1}^{2}\{J(J+1) - [K\pm(n-1)](K\pm n)\}, \\
& b^{2\pm}_{n,v,\ell} = \prod_{n=1}^{n}\{[v+\ell+1)\pm(2n-1)][v-\ell+1\mp(2n-1)]\}, \\
& C^{\mp}_{1} = X_{\ell\ell}(\ell\pm1) + (A-B)_v(K\mp1) - (A\zeta)_v(K+\ell\pm2), \\
& C^{\pm}_{2} = 8X_{\ell\ell}(\ell\pm2) - 4(A-B)_v(K\mp1) - 4(A\zeta)_v(2K-\ell\mp4), \\
& C^{\mp}_{3} = 4X_{\ell\ell}(\ell\mp1) - (A-B)_v(2K\mp1) - 2(A\zeta)_v(\pm2K\mp\ell+2).
\end{aligned}
$$

4. Results and Discussion

Some rotational components were measured for the transitions $\Delta J = 1 \leftarrow 0, \Delta J = 2 \leftarrow 1$ and $\Delta J = 3 \leftarrow 2$, in the range 17–50 GHz for the $\nu_9 = 1$ and the $\nu_{10} = 2$ vibrational states of the ^{13}CH$_3$CCH molecule.

These components are given in Tables 2 and 3, respectively. As a starting point in the frequency search for the rotational components of the $\nu_9 = 1$ vibrational state, the difference between the value of the rotational constant B_{v} for the $\nu_9 = 1$ and value of the rotational constant B_0 for the ground state for the parent species CH_3CCH was considered, ($B\nu_{9=1} - B_0 = 5.178$ MHz) [8]. It was assumed that the rotational constant B_v for $\nu_9 = 1$ will have approximately the same difference from B_0 for the $^{13}CH_3CCH$ isotopomer [11], which gives $B_{\text{v}} = 8318.426$ MHz as a trial value for the $\nu_9 = 1$ vibrational state. Also, as a starting point in the frequency search for the rotational components of the $\nu_{10} = 2$ vibrational states, it was helpful to notice that, for the parent species CH_3CCH [10], both the difference between the rotational constant B_{v} for the ν_{10} =1 vibrational state and B_0 for the ground state ($B\nu_{10=1} - B_0 = 24.1148$ MHz), and the difference between B_{v} for the $\nu_{10} = 2$ vibrations state and B_{v} for the $\nu_{10} = 1$ state ($B\nu_{10=2} - B\nu_{10=1} = 23.96$ MHz), these differences were nearly the same. Therefore it was assumed that the isotopomer $^{13}CH_3CCH$ will follow the same trend. Then by adding the difference between the rotational constant B_{v} for the $\nu_{10} = 1$ vibrational and B_0 for the ground state ($B\nu_{10=1} - B_0 = 23.312$ MHz) for the isotopomer $^{13}CH_3CCH$ [11], to the value $B\nu_{10=1}$ for the isotopomer $^{13}CH_3CCH$, one gets a trial value for the rotational constant $B\nu_{10=2} = 8359.872$ MHz. From table 4, it is obvious that both trial values of B_{v} for the ν_9 =1 and the $\nu_{10} = 2$ vibrational states were proven to be very close to the values found, which gives the best fit between experimental and theoretical values of the frequencies. Some components in Tables 2 and 3 could not be measured. This may be explained by the distortion of the shape of the lines due to the presence of standing waves in the absorption cell around the frequencies expected for them.

Table 2. Some rotational components in the $\nu_9 = 1$ vibrational state of the isotopic species $^{13}CH_3CCH$. All frequencies are in MHz.

J	K	ℓ	ν_{cal}	ν_{obs}	$\Delta\nu$
0	0	±1	16637.455	16637.536	-0.081
1	-1	-1	33243.817	*	*
1	∓1	±1	33272.770	33272.973	-0.203
1	0	±1	33274.799	33274.705	0.094
1	1	1	33307.385	33307.221	0.164
2	∓2	±1	49903.942	49903.221	0.721
2	-1	-1	49865.510	49865.327	0.183
2	∓1	±1	49908.909	49908.712	0.197
2	0	±1	49911.921	49911.817	0.104
2	1	1	49960.862	*	*
2	±2	±1	49912.535	49912.452	0.083

*These frequencies could not be measured.

It is obvious from the theoretical model (Equation 1) that the least deviation between experimental and theoretical frequencies is expected for the components of quantum numbers $K\ell = 0$ in each J level (see Tables 2 and 3). Once these components are assigned, they can serve as a primary determination of the rotational constants for a given vibrational state. Once the other components of major branches have been measured and identified, the rotational constants were refined by iterative techniques. This iterative process is performed to minimize the differences between theoretical and experimental frequencies by varying each constant over a reasonable range in successive iterations using a computer program based on the least squares method [28].

At the beginning of the calculation, all of the parameters for the $\nu_{10} = 2$ vibrational state for the $^{13}CH_3CCH$ isotopic species, except B_{v}, were fixed to the values of the $\nu_{10} = 2$ for the parent species CH_3CCH as trial values [10]. After the iteration process performed, the fixed values of D_J, ζ and q_{v} were proven to be the best ones, while the values of the other parameters (D_{JK}, $\gamma_{\ell\ell}$, η_{J}, η_{JJ}, η_{JK}, A_{v}, $X_{\ell\ell}$, q_{12}, d_{12}) need to be slightly altered to give the best fit between the experimental and theoretical frequencies. The values of all paremeters, except B_{v} and $X_{\ell\ell}$, for the $\nu_9 = 1$ vibrational state for the parent species CH_3CCH [8] were used as trial values for the calculation of the rotational frequencies for the $\nu_9 = 1$ vibrational state for the $^{13}CH_3CCH$ isotopic species. After the iteration process was performed, all of the parameters required alteration to give the best fit between the experimental and theoretical frequencies. The anharmonic constant $X_{\ell\ell}$ was determined by using its value reported for the $\nu_9 = 2$ vibrational state of the parent species CH_3CCH [8] as a trial value, then it was iterated to give the value reported in Table 4, which gives the best fit. Table 4 gives the rotational constants which gives the best fit between theoretical and experimental values of the rotational frequencies for both vibrational states.

Table 3. Some rotational components in the $\nu_{10} = 2$ vibrational state of the isotopic species $^{13}CH_3CCH$. All frequencies are in MHz.

J	K	ℓ	ν_{cal}	ν_{obs}	$\Delta\nu$
0	0	0	16715.534	16715.515	0.019
0	0	±2	16715.270	16715.170	0.100
1	∓1	±2	33425.202	33425.420	-0.218
1	0	0	33430.907	33430.738	0.169
1	0	±2	33430.845	33430.738	0.107
1	±1	0	33430.161	33430.110	0.051
1	±1	±2	33434.132	33434.662	-0.530
2	∓2	±2	50119.936	*	*
2	∓1	±2	50133.693	50133.024	0.669
2	0	0	50145.959	50145.789	0.170
2	0	±2	50147.030	50146.844	0.186
2	±1	0	50144.789	50144.526	0.263
2	±1	±2	50154.802	*	*
2	±2	0	50141.189	*	*
2	±2	±2	50162.925	50163.673	-0.748

*These frequencies could not be measured

Table 4. The rotational constants for the $\nu_9 = 1$ and the $\nu_{10} = 2$ vibrational states of the isotopic species $^{13}CH_3CCH$. All constants are in MHz, except ζ is dimensionless.

Constant	$\nu_9 = 1$	$\nu_{10} = 2$
B_{v}	$8318.736\underline{0}$	$8358.035\underline{0}$
$\gamma_{\ell\ell}$	0.0	$-0.12\underline{6}4$
D_{JK}	$0.159\underline{7}$	$0.164\underline{3}$
η_{J}	$0.365\underline{2}$	$0.335\underline{3}$
η_{JK}	0.0	0.01
D_J	$0.0035\underline{9}$	$0.0031\underline{2}$
η_{JJ}	0.0	$0.0\underline{3}$
ζ	$0.98\underline{4}$	$0.88\underline{9}$
q_V	$3.97\underline{3}$	$4.18\underline{5}8$
$X_{\ell\ell}$	$14\underline{7}000$	$14\underline{7}800$
A_{v}	$15\underline{5}000$	$15\underline{4}000$
q_{12}	$1\underline{1}.0$	$-3\underline{3}.0$
d_{12}	0.0	$11\underline{2}.0$

Note: the last statistically significant digit for each constant is underlined.

The values, to the last statistically significant digit, of the rotational constant A_{v} for the $\nu_9 = 1$ and the $\nu_{10} = 2$ vibrational states (see Table 4) were found to agree with the values reported by Pekkala et al. [18] for CH_3CCH, at 159100 MHz and 158900 MHz for the $\nu_9 = 1$ and the $\nu_{10} = 2$ vibrational states, respectively. Table 5 gives a comparison of the value of the rotational parameters of each of the $\nu_9 = 1$ and the $\nu_{10} = 2$ vibrational states and their corresponding values for the $\nu_{10} = 1$ reported by Tam et al. [11] for the same isotopic species $^{13}CH_3CCH$. From the comparison, the differences for D_J,D_{JK} and q_v were found to be of the same order as the differences reported in [18] for the parent species CH_3CCH, while the other parameters were found to be comparable to the values reported in reference [10] for the parent species.

Good agreement was found between the experimental and theoretical values for most components; except for the components of quantum numbers ($K\ell$ = -2) for each J in the $\nu_9 = 1$ vibrational state, and the components of quantum numbers ($K \neq 0, \ell = \pm 2$) for each J in the $\nu_{10} = 2$ vibrational state, showing departure between the experimental and theoretical values. This may be attributed to a Fermi resonance between the $\nu_9 = 1$ and the $\nu_{10} = 2$ vibrational states as suggested by Pekkala et al. [18] for the parent species CH_3CCH, and by Schroderus et al. [20] for the isotopic species CD_3CCD.

Table 5. A Comparison of some parameters of each of the $\nu_9 = 1$ and the $\nu_{10} = 2$ vibrational states with the $\nu_{10} =$ 1 vibrational state for the isotopic species $^{13}CH_3CCH$. All parameters are in MHz, except ζ is dimensionless.

Constant	Δ_1*	Δ_2**
D_{JK}	3.9×10^{-3}	8.5×10^{-3}
η_J	3.22×10^{-2}	2.3×10^{-3}
η_{JK}	0	1×10^{-2}
D_J	$-9 x10^{-5}$	-5.6×10^{-4}
η_{JJ}	0	3×10^{-2}
ζ	1.04×10^{-1}	9×10^{-3}
q_V	-1.8×10^{-2}	1.95×10^{-1}
A_v	1×10^1	1.6×10^1

*Δ_1 = the value of the parameter of $\nu_9 = 1$ (Table 4) − its value for the $\nu_{10} = 1$ reported in reference 11.
**Δ_2 = the value of the parameter of $\nu_{10} = 2$ (Table 4) − its value for the $\nu_{10} = 1$ reported in reference 11.

5. Conclusion

In this work some rotational components in the $\nu_9 = 1$ and the $\nu_{10} = 2$ vibrational states were measured for the first time for the isotopomer $^{13}CH_3CCH$ in the microwave region. A set of rotational constants for both the $\nu_9 = 1$ and the $\nu_{10} = 2$ vibrational states was determined, which gives the best fit between the experimental and theoretical values; except for the components of of quantum numbers ($K\ell = -2$) for each J in the $\nu_9 = 1$ and of quantum numbers ($K \neq 0, \ell = \pm 2$) for each J in the $\nu_{10} = 2$ vibrational states respectively. This departure was attributed to a Fermi resonance between these two vibrational states.

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