

Microwave Spectra of $^{13}\text{CH}_3^{15}\text{N}$ and $^{13}\text{CH}_3^{13}\text{C}^{15}\text{N}$ Molecules In the Frequency Range 17-95 GHz

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طيف الميكروويف لجزيئات $^{13}\text{CH}_3^{15}\text{N}$ and $^{13}\text{CH}_3^{13}\text{C}^{15}\text{N}$ مدى التردد من ١٧ - ٩٥ جيجا هيرتز

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بعض ترددات الميكروويف للنظيرين $^{13}\text{CH}_3^{15}\text{N}$ and $^{13}\text{CH}_3^{13}\text{C}^{15}\text{N}$ من ميثايل السيانيد في مدى التردد الاهتزازي للمركبة $\nu_7 + \nu_8$ قد قيست في النطاق الترددي ما بين 17-95 GHz للنتقالات $\Delta J = 1 \leftarrow 0, \Delta J = 2 \leftarrow 1, \Delta J = 3 \leftarrow 2, \Delta J = 5 \leftarrow 4$.

هذا وقد توافقت جيد بين التجارب العملية والقيم النظرية المتوقعة لمركبات الأعداد الكمية $k = \nu = \pm 1$ لكل J.

هذه المركبات أظهرت فرق شاسع بين النتائج النظرية والنتائج العملية والتي ساهمت في نوعين من رنين فيرمي للحالات الاهتزازية ما بين ν_3 و $\nu_7 + \nu_8$ و ν_6 و $\nu_7 + \nu_8$.

Key Words: Microwave Spectra - $^{13}\text{CH}_3^{15}\text{N}$ - $^{13}\text{CH}_3^{13}\text{C}^{15}\text{N}$ - frequency range.

ABSTRACT

Some microwave frequencies of the $\nu_7 + \nu_8$ vibrational combination band for the two isotopes $^{13}\text{CH}_3^{15}\text{N}$ and $^{13}\text{CH}_3^{13}\text{C}^{15}\text{N}$ of methyl cyanide were measured in the frequency range 17-95 GHz, for the transitions $\Delta J = 1 \leftarrow 0, \Delta J = 2 \leftarrow 1, \Delta J = 3 \leftarrow 2, \Delta J = 5 \leftarrow 4$. Good agreement was found between experimental and theoretical values except for the components of quantum numbers $k = \nu = \pm 1$ for each J. These components show a large departure between experimental and theoretical values, which attribute to two fermi resonances between ν_3 and $\nu_7 + \nu_8$, also between ν_6 and $\nu_7 + \nu_8$ vibrational states.

1. Introduction

Methyl Cyanide molecule (CH_3CN) is a prolate symmetric top molecule with a large dipole moment ($\mu = 3.91\text{D}$)[1-3]. It is a very abundant species in the interstellar medium and is an ideal observational probe of the kinetic temperature and density of interstellar clouds [4,5]. It is one of the molecular species, which have been definitely identified in the atmosphere of Titan, Jupiter and Saturn [6,7]. Recently, it is identified in the coma of Comet 1P/Halley [8]. For these reasons many studies have been devoted to investigate its molecular spectra and molecular structure in the microwave region [9-16] and in the infrared region [17-26]. Johri *et al* [9] and Al-Share *et al* [10] have studied the fermi resonance between the ν_7 and the $3\nu_8$ vibrational states for the ^{13}C and ^{15}N tagged isotopes. Tam *et al* [13] and Tam and Roberts [14] have studied the rotational spectra for the ^{13}C isotopes of CH_3CN in the ground, ν_8 , $2\nu_8$ vibrational levels. Sabeih *et al* [15] have studied the rotational spectra for $\text{CH}_3\text{C}^{15}\text{N}$ isotope in the ground, ν_8 , $2\nu_8$ and $3\nu_8$ vibrational levels. Al-Share [16] has measured the rotational components for the hot band $\nu_8 + \nu_8 - \nu_8$ for the two isotopes $^{13}\text{CH}_3\text{C}^{15}\text{N}$ and $^{13}\text{CH}_3\text{C}^{13}\text{C}^{15}\text{N}$.

Duncan *et al* [17] had reported, in their infrared spectrum, a fermi resonance between the ν_7 and the $3\nu_8$ vibrational levels and the ν_6 and the combination band $\nu_7 + \nu_8$. Matsuura *et al* [18] and Mori *et al* [19] have studied the ν_6 band and the combination band $\nu_7 + \nu_8$ region and reported a fermi resonance between them. A. M. Tolonen *et al* [20] have studied the ν_7 and the ν_4 , the fermi resonance between ν_7 and $3\nu_8^1$ the t-type resonance between the ν_7^1 and the ν_7^{-1} and the fermi resonance between ν_7 and $2\nu_8^2$. Koivusaari *et al* [21] and Antilla *et al* [22] have studied the infrared spectra of the ν_8 and the combination band $\nu_7 + \nu_8$ and the hot band $\nu_7 + \nu_8 - \nu_8$ of the parent molecule $^{12}\text{CH}_3\text{C}^{12}\text{C}^{14}\text{N}$. Paso *et al* [23] have studied the region covers the ν_3 , ν_6 and $\nu_7 + \nu_8$ for $^{12}\text{CH}_3\text{C}^{12}\text{C}^{14}\text{N}$ and reported a fermi resonance between ν_6 and $\nu_7 + \nu_8$ and between ν_3 and $\nu_7 + \nu_8$.

As can be seen from figure (1), which shows the energy levels for the ν_3 , ν_6 and $\nu_7 + \nu_8$ vibrational modes for the parent molecule $^{12}\text{CH}_3\text{C}^{12}\text{C}^{14}\text{N}$ and the two isotopes $^{13}\text{CH}_3\text{C}^{15}\text{N}$ and $^{13}\text{CH}_3\text{C}^{13}\text{C}^{15}\text{N}$, the band center for the $\nu_7 + \nu_8$ combination band was reported to be 1408.933 cm^{-1} for the parent molecule [23]. Using the effect of isotopic substitution ^{13}C and ^{15}N on the value of the ν_7 and the ν_8 as reported by Duncan *et al* [17], the value of the band center for the combination band $\nu_7 + \nu_8$ was calculated to be 1397.733 cm^{-1} and 1385.393 cm^{-1} for $^{13}\text{CH}_3\text{C}^{15}\text{N}$ and $^{13}\text{CH}_3\text{C}^{13}\text{C}^{15}\text{N}$ respectively. In this paper, some rotational components for the combination band $\nu_7 + \nu_8$ for the two isotopes $^{13}\text{CH}_3\text{C}^{15}\text{N}$ and $^{13}\text{CH}_3\text{C}^{13}\text{C}^{15}\text{N}$ will be measured using the microwave spectrometer, and a set of rotational constants will be given for the first time of the combination band $\nu_7 + \nu_8$ for these two isotopes, and to utilize the method of isotopic substitution in tuning the molecule internally by bringing the vibrational levels ν_7 , ν_6 and $\nu_7 + \nu_8$ more closely, which makes the interactions between them stronger.

Experimental Details

The measurements reported in this work were made using the microwave spectrometer that was described earlier [12,26]. Figure (2) shows a block diagram of it. The sensitivity of the instrument is quite high with

a cylindrical absorption cell of 60-m length. The cell was excited by a rectangular to circular feed horn and detection achieved reciprocally. The spectral profiles were displayed on a dual pen chart recorder with one pen producing the frequency markers and the other pen producing the spectral line profiles. Figure (3), shows a typical scan of the spectral profile $\Delta j = 2 \leftarrow 1$ rotational transition of the vibrational combination band $\nu_7 + \nu_8$ for $^{13}\text{CH}_3\text{C}^{15}\text{N}$ isotope.

Even though the components of the $\nu_7 + \nu_8$ is somewhat stronger than of the $\nu_7 + \nu_8$ [21], these lines resolution became difficult and a series of runs had to be made to pressurize and depressurize the cell with a gas sample until the resonance profile could be identified. The use of the chart recording allows for long-term scanning over only a few MHz. The scan rate used in this work was 1MHz per min, thus allowing good signal integration and noise filtering over the interval. From figure 3, one can see how the chart-recorded signals may be measured. 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 interval scales the frequency interval. These marker ticks recorded by the second pen of the dual-pen chart recorder, as can be seen in the margin of figure 3, and they serve to partition the frequency interval and establish the absolute frequency. Once 10 or more scans have been acquired for each line, the structure of each line derivative is studied for symmetry and frequency position along the interval. Two or more independent sets of data are taken for each spectral line before the data are considered to be complete. If overall repeatability is less than 50 KHz, the spectral line is assumed to be satisfactorily measured.

Commercial sample of $^{13}\text{CH}_3\text{C}^{15}\text{N}$ which was 99% enriched with ^{13}CH and ^{15}N atoms respectively. They were obtained from Merck Frosst Canada Inc. [26]. Each sample was frozen under vacuum conditions and any extra gases were pumped away using a cold-tapped diffusion pump vacuum in the standard way. Calibrated samples of 1-2 mTorr of vapor were admitted into the vacuum chamber as wanted for each run of measurements.

Theoretical Formula

A theoretical model was used in the present work for the calculations of frequencies of rotational transitions $J + 1 \leftarrow J$ which was derived by Rhee and Roberts [27] is given here in a new form, with the symbols have their usual meaning as given elsewhere [10], but they will be given here for convenience, B_v and A_v are the principal rotational constants, X_{ii} is the anharmonic constant, ζ is the coriolis coupling constant, D_J , D_{JK} D_K are the first order centrifugal distortion constants $\gamma_u = B_3$ is coriolis centrifugal stretch constant η_j , η_{JJ} , η_{JK} , η_{KK} are the higher order diagonal matrix elements.

$$\begin{aligned} \nu(\nu, J, K, l) = & 2(J+1) \{ [B_v + \gamma_{ll} l^2 - D_{JK} k^2 - 2D_J (J+1)] \\ & + [\eta_J K l + \eta_{JK} K^3 l + 2\eta_{JJ} K l (J+1)] \\ & \pm [q_v (V+1)_{kl=\pm 1} + f_{24} \nu(\nu+2)_{\substack{k=\pm 1 \\ l=\pm 2}}] \} \\ & \pm [b_{1v,l}^{\pm} / C_1^{\pm}]_{kl \neq 1} q_v^2 + (b_{2v,l}^{\pm} / C_2^{\pm})_{kl \neq 2} f_{24}^2 \end{aligned}$$

$$\begin{aligned}
 & [a_2, J^{2 \pm} + 1, K^{-a_2}, J^{2 \pm}, K] \pm (b_1, v^{2 \pm}, \ell / C_3^{\pm}) \\
 & [a_1, J^{2 \pm} + 1, K^{-a_1}, J^{2 \pm}, K] [q_{12}(2K \pm 1) + d_{12}(\ell \pm 1)]^2 \quad \text{Eq. (1)}
 \end{aligned}$$

Where:

$$\begin{aligned}
 a_n, J^{2 \pm}, K &= \prod_{n=1}^n \{J(J+1) - [K \pm (n-1)](K \pm n)\} \\
 b_n, v^{2 \pm}, \ell &= \prod_{n=1}^n \{[v + \ell + 1] \pm (2n - 1)[v - \ell + 1 \mp (2n - 1)]\} \\
 C_1^{\pm} &= X_{\ell} \{(\ell \pm 1) + (A - B)_v(K \pm 1) - (A\zeta)_v(K + \ell \pm 2)\} \\
 C_2^{\pm} &= 8 X_{\ell} \{(\ell \pm 2) - 4(A - B)_v(K \mp 1) - 4(A\zeta)_v(2K + \ell \pm 4)\} \\
 C_3^{\pm} &= 4 X_{\ell} \{(\ell \pm 1) - (A - B)_v(2K \mp 1) - 2(A\zeta)_v(\pm 2K \mp \ell \pm 4)\}
 \end{aligned}$$

Results and Discussion

In this work 60 rotational components were measured for the transitions $\Delta J = 0 \leftarrow -1$, $\Delta J = 2 \leftarrow -1$, $\Delta J = 3 \leftarrow -2$, $\Delta J = 5 \leftarrow -4$ which assigned to the $v_7 + v_8$ combination band for the two isotopes $^{13}\text{CH}_3^{15}\text{N}$ and $^{13}\text{CH}_3^{13}\text{C}^{15}\text{N}$. As a starting point in the frequency search for the rotational components of the $v_7 + v_8$ combination band, the difference between the rotational constant B_v for the $v_7 + v_8$ band and B_0 for the ground vibrational state was considered, which was 23.2639 MHz for the parent molecule $^{12}\text{CH}_3^{12}\text{C}^{14}\text{N}$ [23]. So, it was assumed that the two isotopes $^{13}\text{CH}_3^{15}\text{N}$ and $^{13}\text{CH}_3^{13}\text{C}^{15}\text{N}$ will follow the same trend. This assumption was proven to be correct, since the difference between the rotational constant ($B_v = 8683.846$ MHz) and B_0 for the ground state ($B_0 = 8659.866$ MHz [13]) was found to be 24.98 MHz for isotope $^{13}\text{CH}_3^{15}\text{N}$, also the difference between the rotational constant B_v for the $v_7 + v_8$ band ($B_v = 8677.853$ MHz) and B_0 for the ground state ($B_0 = 8655.903$ MHz [13]) was found to be 21.95 MHz for the isotope $^{13}\text{CH}_3^{13}\text{C}^{15}\text{N}$, both differences were close to that, mentioned above, for $^{12}\text{CH}_3^{12}\text{C}^{14}\text{N}$.

A systematic study of the frequency of each component of the $v_7 + v_8$ combination band was undertaken to establish a trend in the variation of the predicted values of frequency for each rotational line from the experimental measured values. From the theoretical model (equation 1), it is obvious that the least deviation between experimental and theoretical frequencies is expected for the $K = \ell = 0$ components in each J level, also see tables (1) and (2). Experimental values can be taken from these transitions, once they are assigned, to best express the rotational constants for a given vibrational state. Once measurements and identification of the non-assigned lines of major branches was made, the constants for the other branches were approximated and refined by iterative techniques. This iterative process is performed to minimize the differences between the measured frequencies and those calculated from equation 1, by varying each constant over a reasonable range. The rotational constants set obtained, see table 3, was refined in a successive iterations using a computer program based on the least square method [9, 16].

Table (1) gives 30 rotational components which were measured for the transitions $\Delta J = 1 \leftarrow 0$, $\Delta J = 2 \leftarrow 1$, $\Delta J = 3 \leftarrow 2$, $\Delta J = 5 \leftarrow 4$, which cover the range of 17-87 GHz of the $v_7 + v_8$ band for the isotope $^{13}\text{CH}_3^{15}\text{N}$.

Also, table (2) gives 30 rotational components of the $\nu_7 + \nu_8$ band for the isotope $^{13}\text{CH}_3^{13}\text{C}^{15}\text{N}$. Good agreement between the theoretical calculated and experimental measured values was found, and the departure found for $K = \tau = \pm 1$ components are attributed to both fermi resonances between the ν_6 and the $\nu_7 + \nu_8$ vibrational states, since this departure found for $K = \tau = \pm 1$ components was not symmetrical, as seen from tables (1 and 2), which means that more than one interaction are at play [23].

Table (3) gives the rotational constants set for the $\nu_7 + \nu_8$ combination band for both isotopes $^{13}\text{CH}_3^{13}\text{C}^{15}\text{N}$ and $^{13}\text{CH}_3^{13}\text{C}^{15}\text{N}$, which gives the best fit between the experimental and theoretical values using a fitting computer program based on the least square method [9, 16].

Conclusion

In this work 60 rotational components of the $\nu_7 + \nu_8$ combination band were measured for the first time for both isotopes $^{13}\text{CH}_3^{13}\text{C}^{15}\text{N}$ and $^{13}\text{CH}_3^{13}\text{C}^{15}\text{N}$. Also 13 rotational parameters were determined of the $\nu_7 + \nu_8$ combination band for the above two isotopes. Good agreement was found for the components of the $\nu_7 + \nu_8$ combination band except for the components of quantum number set $K = \tau = \pm 1$ of each J value in the. This departure was due to a fermi resonance between the ν_6 and the $\nu_7 + \nu_8$ vibrational states and between the ν_3 and the $\nu_7 + \nu_8$ vibrational states as suggested by Paso et al [23]. Also, the molecule was, successfully, tuned internally using the method of isotopic substitution by bringing the vibrational states closer and making the interactions stronger.

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Table 1: Some rotational components in the $\nu_7 + \nu_8$ vibrational combination band of the isotope $^{13}\text{CH}_3\text{C}^{15}\text{N}$. All frequencies are in MHz.

| J | K | ι | ν_{cal} | ν_{obs} | $\Delta\nu$ |
|---|---------|---------|--------------------|--------------------|-------------|
| 0 | 0 | ± 1 | 17369.993 | 17369.981 | 0.012 |
| 1 | -1 | -1 | 34717.325 | 34709.639 | 7.686 |
| 1 | ± 1 | ± 1 | 34737.59 | 34737.263 | 0.326 |
| 1 | 0 | ± 1 | 34739.874 | 34739.825 | 0.049 |
| 1 | 1 | 1 | 34764.077 | 34773.555 | -9.478 |
| 2 | ± 2 | ± 1 | 52099.066 | | |
| 2 | -1 | -1 | 52075.898 | 52066.781 | 9.117 |
| 2 | ± 1 | ± 1 | 52106.003 | 52106.254 | -0.251 |
| 2 | 0 | ± 1 | 52109.533 | 52109.593 | -0.060 |
| 2 | 1 | 1 | 52146.026 | 52157.366 | -11.340 |
| 2 | ± 2 | ± 1 | 52111.251 | 52111.126 | 0.125 |
| 4 | ± 4 | ± 1 | 86780.264 | 86780.694 | -0.430 |
| 4 | ± 3 | ± 1 | 86809.354 | 86809.065 | 0.289 |
| 4 | ± 2 | ± 1 | 86829.089 | | |
| 4 | -1 | -1 | 86792.690 | 86781.469 | 11.221 |
| 4 | ± 1 | ± 1 | 86841.304 | 86841.542 | -0.238 |
| 4 | 0 | ± 1 | 86847.740 | 86847.784 | -0.044 |
| 4 | 1 | 1 | 86909.570 | 86923.288 | -13.718 |
| 4 | ± 2 | ± 1 | 86852.619 | 86852.890 | -0.271 |
| 4 | ± 3 | ± 1 | 86853.356 | 86852.890 | -0.534 |
| 4 | ± 1 | ± 1 | 856.071 | | |

Table 2: Some rotational components in the $\nu_7 + \nu_8$ vibrational combination band of the isotope $^{13}\text{CH}_3^{13}\text{C}^{15}\text{N}$. All frequencies are in MHz.

| J | K | ι | ν_{cal} | ν_{obs} | $\delta\nu$ |
|---|---------|---------|--------------------|--------------------|-------------|
| 0 | 0 | ± 1 | 17355.926 | 17355.975 | -0.049 |
| 1 | -1 | -1 | 34692.045 | 34681.234 | 10.811 |
| 1 | ± 1 | ± 1 | 34709.490 | 34709.324 | 0.166 |
| 1 | 0 | ± 1 | 34711.739 | 34711.751 | -0.012 |
| 1 | 1 | 1 | 34732.365 | 34746.194 | -13.829 |
| 2 | ± 2 | ± 1 | 52056.967 | 52057.145 | -0.178 |
| 2 | -1 | -1 | 52037.912 | 52026.296 | 11.616 |
| 2 | ± 1 | ± 1 | 52063.909 | | |
| 2 | 0 | ± 1 | 52067.326 | 52067.367 | -0.041 |
| 2 | 1 | 1 | 52098.392 | 52112.457 | -14.065 |
| 2 | ± 2 | ± 1 | 52066.998 | 52066.838 | 0.160 |
| 4 | ± 4 | ± 1 | 86713.133 | | |
| 4 | ± 3 | ± 1 | 86740.511 | 86740.415 | 0.096 |
| 4 | ± 2 | ± 1 | 86759.533 | 86759.627 | -0.094 |
| 4 | -1 | -1 | 86729.022 | 86715.379 | 13.643 |
| 4 | ± 1 | ± 1 | 86771.439 | 86771.282 | 0.157 |
| 4 | 0 | ± 1 | 86777.376 | 86777.623 | -0.247 |
| 4 | 1 | 1 | 86829.822 | 86844.962 | -15.140 |
| 4 | ± 2 | ± 1 | 86778.167 | 86777.623 | 0.544 |
| 4 | ± 3 | ± 1 | 86774.204 | | |
| 4 | ± 4 | ± 1 | 86769.610 | 86769.897 | -0.287 |

Table 3: Some rotational components in the $\nu_7 + \nu_8$ vibrational combination band of the isotope $^{13}\text{CH}_3\text{C}^{15}\text{N}$ and $^{13}\text{CH}_3\text{C}^{13}\text{C}^{15}\text{N}$. All frequencies are in MHz except ζ .

| CONSTANT | $^{13}\text{CH}_3\text{C}^{15}\text{N}$ | $^{13}\text{CH}_3\text{C}^{13}\text{C}^{15}\text{N}$ |
|-------------|---|--|
| B_v | 8684.846 | 8677.853 |
| γ_u | 0.158 | 0.118 |
| D_{JK} | 0.188 | 0.228 |
| η_j | 0.341 | 0.31 |
| η_{JK} | 0.031 | 0.021 |
| D_j | 0.00368 | 0.0038 |
| η_{JJ} | 0.0022 | 0.0012 |
| ζ | 0.886 | 0.896 |
| q_0 | 2.922 | 20520 |
| X_u | 166000 | 165000 |
| A_v | 155000 | 152000 |
| q_{12} | 6.0 | 8.0 |
| d_{12} | 14.0 | 16.0 |

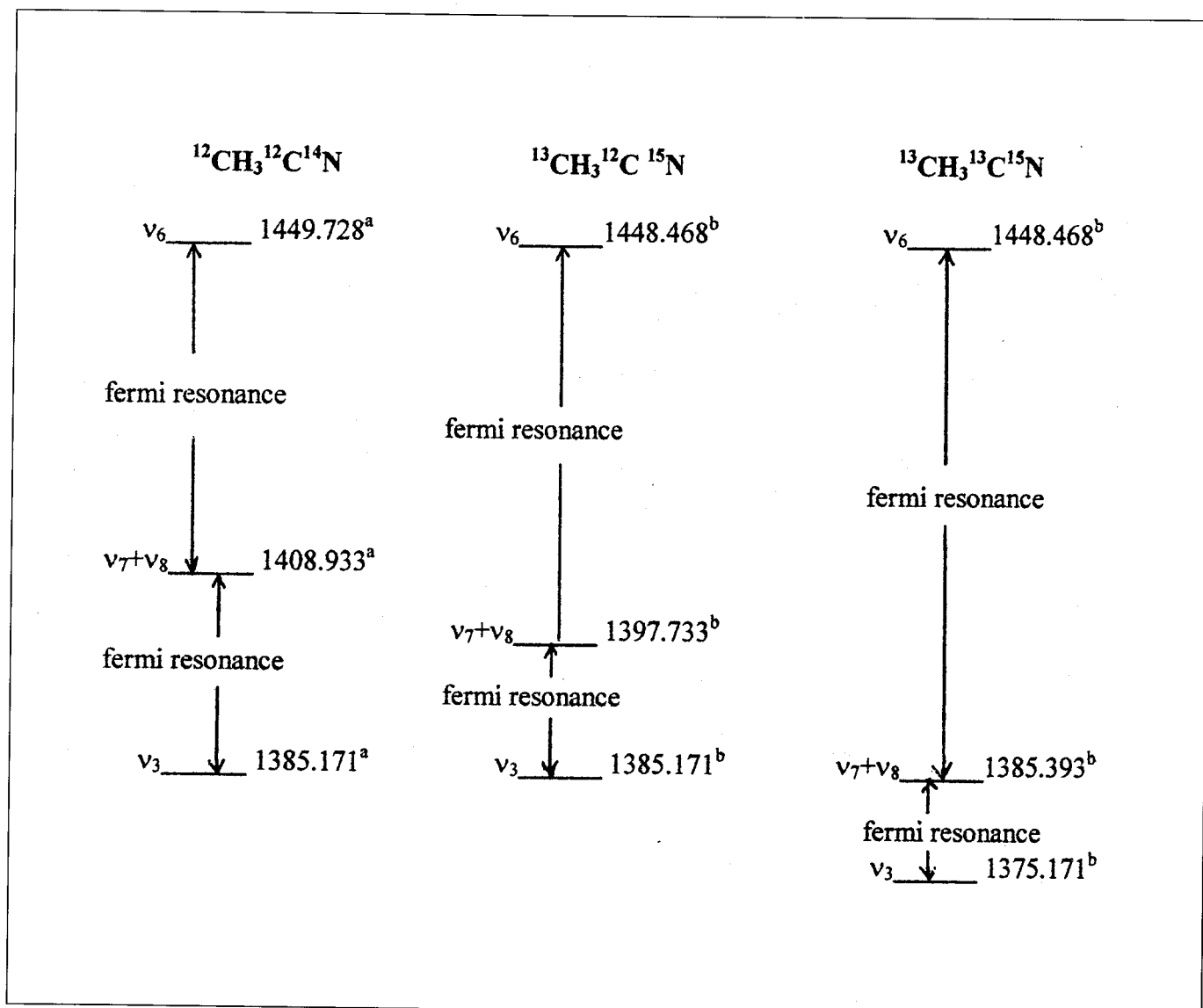


Figure 1 : The energy levels of the v_3 , v_6 and $v_7 + v_8$ vibrational modes of $^{12}\text{CH}_3^{12}\text{C}^{14}\text{N}$, $^{13}\text{CH}_3^{12}\text{C}^{15}\text{N}$ and $^{13}\text{CH}_3^{13}\text{C}^{15}\text{N}$ isotopes. And the Fermi resonance between them.

a) measured from reference 23.

b) estimated values by considering the effect of isotopic substitution ^{13}CH and ^{15}N .

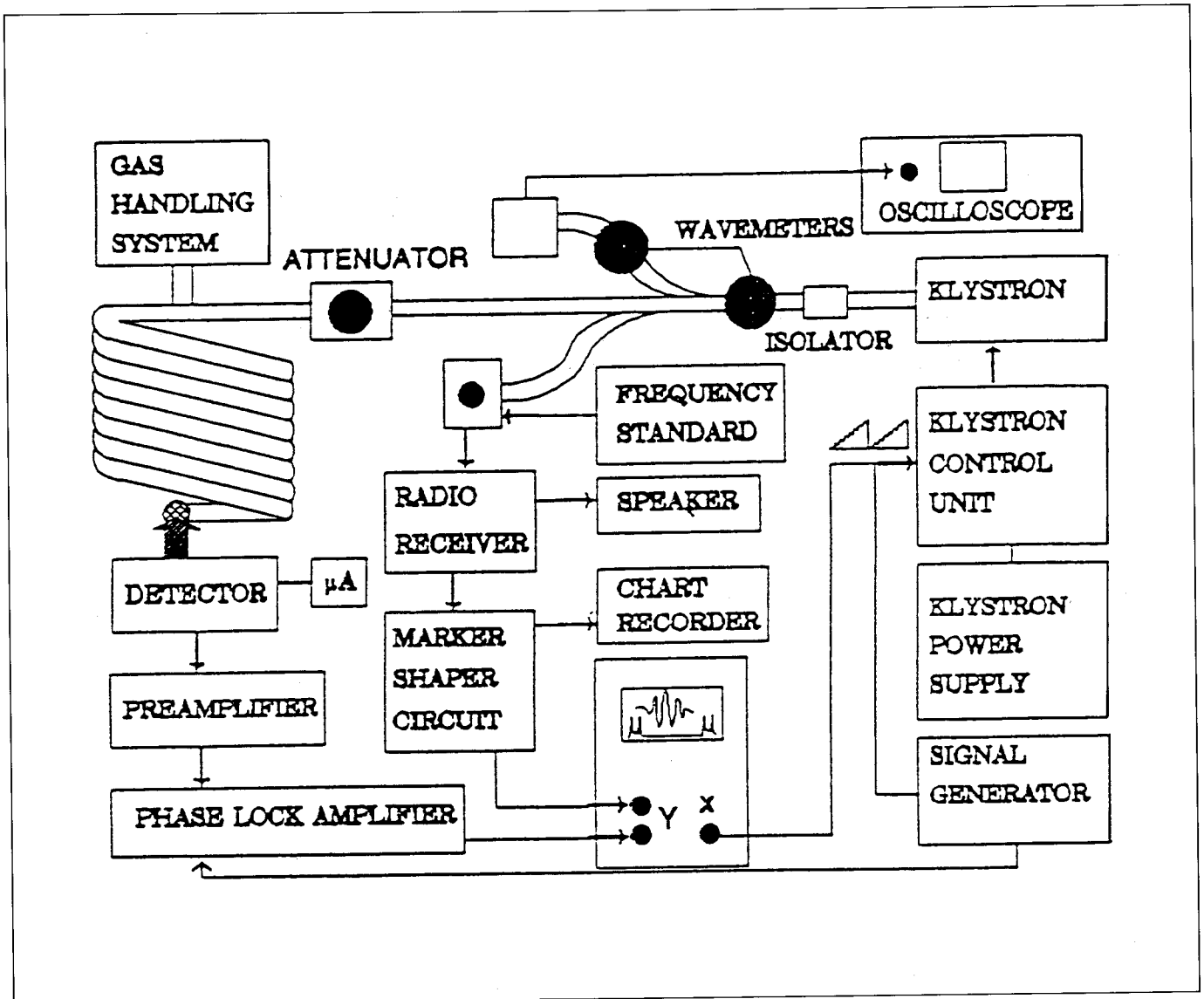


Figure 2 : A block diagram of the spectrometer used to make the measurements reported in this work.

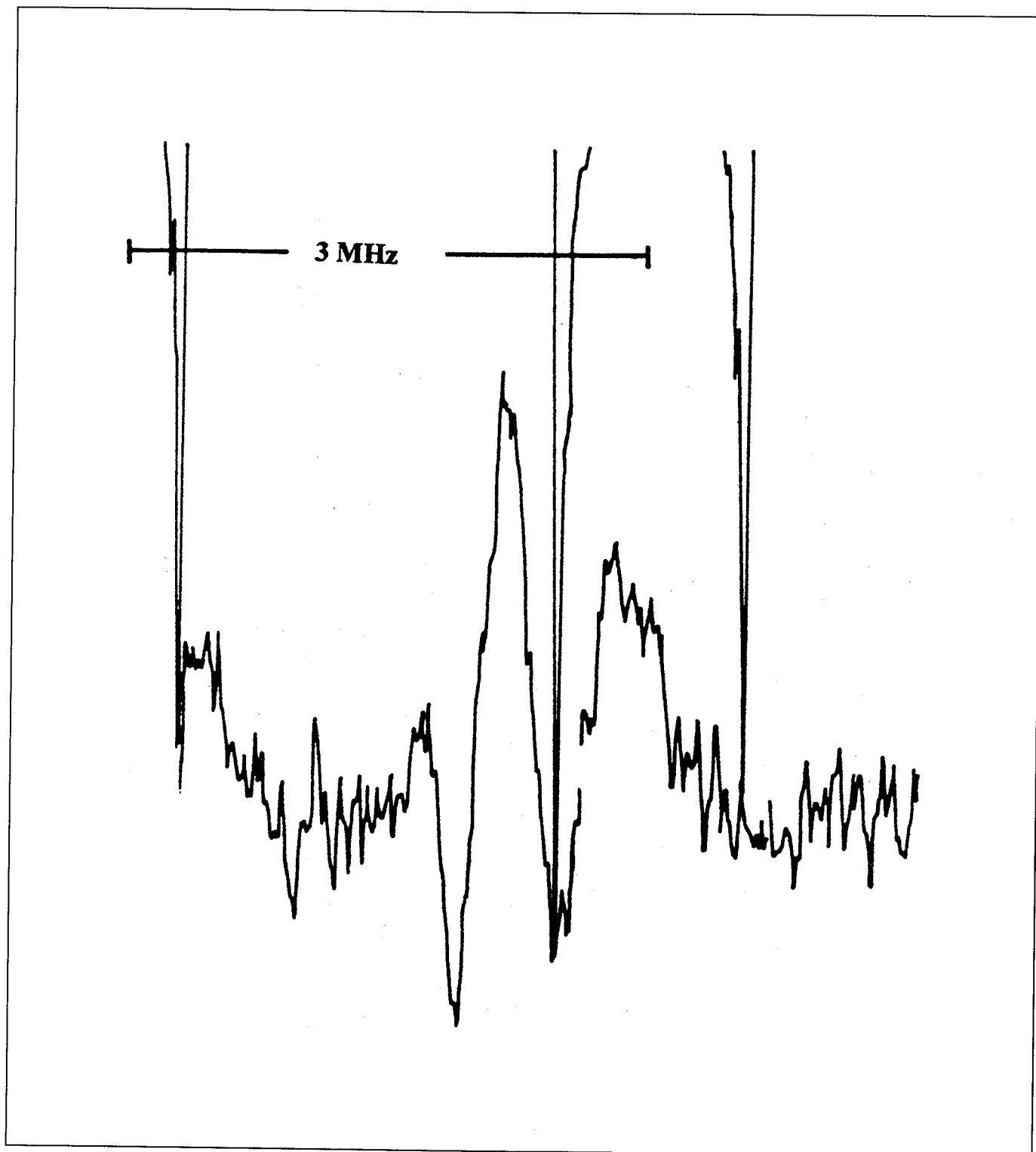


Figure 3 : Dual pen chart recorder trace of some $\Delta J = 3 \leftarrow 2$ rotational components of the $\nu_7 + \nu_8$ vibrational mode of $^{13}\text{CH}_3^{12}\text{C}^{15}\text{N}$. Also the marker ticks are shown.