The Millimeter Wave Spectrum of DCNO: An Example of Current Measurements in the Frequency Range from 60 to 350 GHz

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An efficient system for preliminary data reduction is described which completes a recently developed data acquisition and reduction system for the measurement of millimeter wave absorption lines with the help of a dedicated computer. A simple method of automatically determining the absorption line centers is given.

Rotational transitions of DCNO, measured with the above system, are reported for the ground state and the first excited state of each of the two bending modes ν_4 and ν_5. The rotational and rotation-vibration constants obtained for these states are

$$\begin{aligned} B_0 &= 10{,}292.48340(31)\ \text{MHz}, & D_0 &= 3.5418(10)\ \text{kHz},\\ B_{v_4} &= 10{,}306.00780(45)\ \text{MHz}, & D_{v_4} &= 3.6409(22)\ \text{kHz},\\ B_{v_5} &= 10{,}338.65942(32)\ \text{MHz}, & D_{v_5} &= 3.6208(16)\ \text{kHz}. \end{aligned}$$

The l-type doubling constants $q_t^{(0)}$ and $q_t^{(1)}$ agree with the values obtained previously from direct l-type doubling transitions.

I. Introduction

The rotational spectra of HCNO and DCNO, normal and deuterated fulminic acid, in the microwave region have been reported previously[1–3] together with resulting information concerning the molecular structure and the rotational constants for several excited states. An anomalous dependence of the α_5 value and of the l-type doubling constant q_5 on the vibrational quantum number v_5 was found for both HCNO and DCNO. Subsequently centrifugal distortion effects[4] and the spectra of molecules in excited vibrational states[5] were further investigated by measuring the millimeter wave spectrum of HCNO using a millimeter wave spectrometer with a dedicated computer[6].

Since the measurement and assignment of the far infrared spectrum of HCNO and DCNO[7], it is now possible to interpret some of the anomalous effects observed in the rotational spectrum of both molecules on the basis of a quasilinear molecular model. One of the important remaining steps in the experimental study of the spectrum of fulminic acid was thus the measurement of the millimeter wave spectrum of DCNO for molecules in the ground state and excited vibrational states. We report in this paper our measurements of rotational transitions of DCNO in the ground state and in the first excited state of each of the two bending vibrations ν_4 and ν_5. Data for molecules in higher excited states will be reported separately[8].

Our measurement technique has undergone considerable evolution within the last few years. Since computer oriented measurements are being increasingly often compared as spectroscopists seek to optimize the use of financial resources, equipment and the time of the experimenter, we have devoted the first part of this paper (Sect. II) to a presentation of our current mode of measurement, with emphasis on extensions of the use of a dedicated computer to increase accuracy, reliability and speed of data acquisition and reduction.

In Sect. III we report the measurements of the millimeter wave spectrum of DCNO. These data were analysed in the same manner as the data for HCNO as described in Ref.[4] in order to obtain constants defined in the context of a linear molecular model. In Sect. IV we compare the constants so obtained with those obtained for HCNO, and discuss the usefulness of the quasilinear molecular model in interpreting some of the constants.

II. Current On-line Data Acquisition Techniques for Millimeter Wave Measurements

The basic experimental set-up for millimeter wave measurements has been described previously[6] and a condensed diagram of the spectrometer is shown in Fig.1, which outlines the hardware aspects of the

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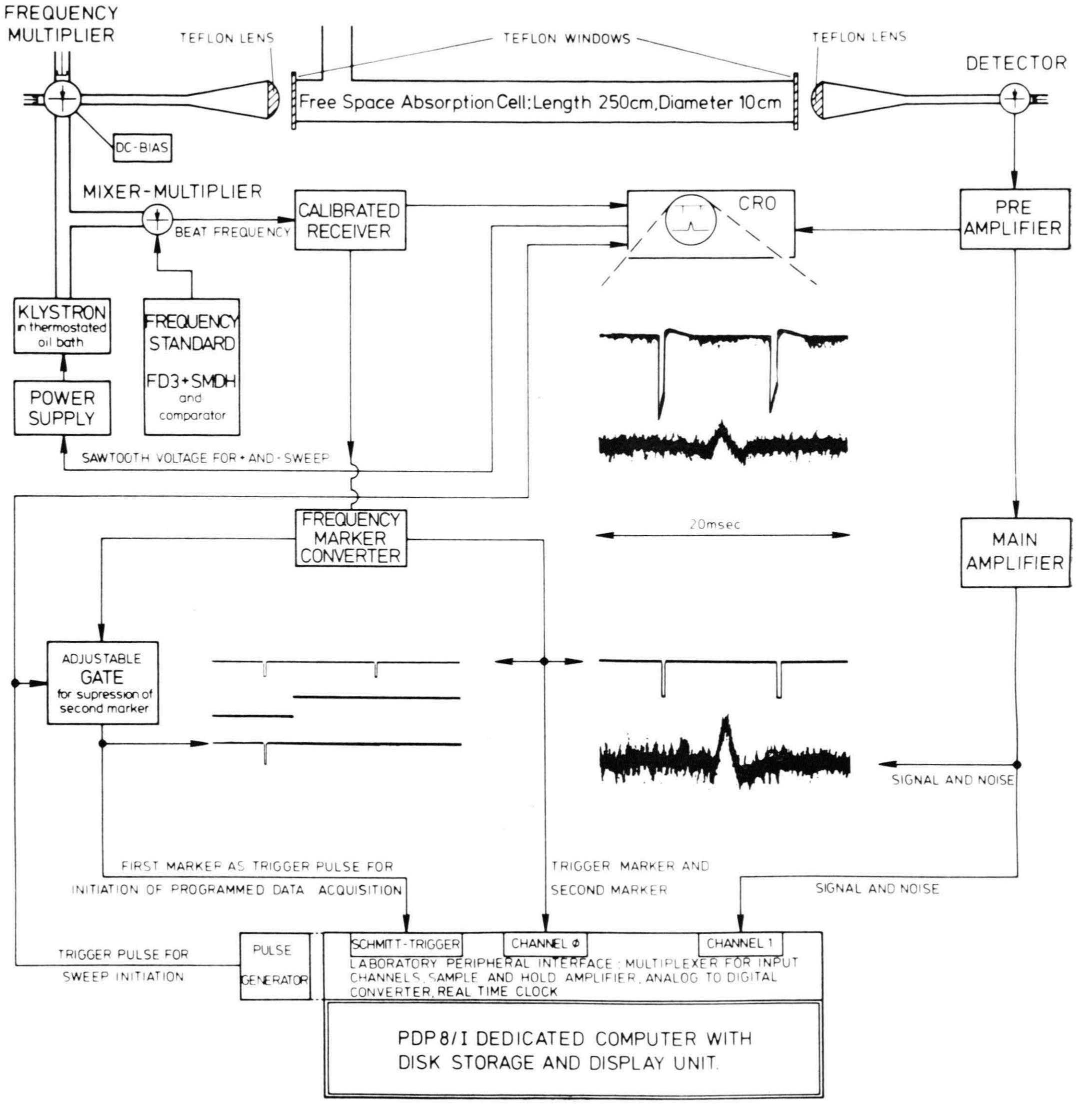


Fig. 1. Hardware aspects of the data acquisition system developed for use with a millimeter wave spectrometer.

preparation of the signal for data acquisition. A conventional millimeter wave video spectrometer supplies the absorption signal which is fed after several stages of amplification into an analog-digital converter attached to a PDP-8/I computer. The computer configuration includes the main unit with a core storage of 8 K and 12 bit word length, a laboratory peripheral interface, a 32 K random access disk, a teletype and a display unit. The application of this system to the basic task of signal averaging to increase sensitivity and accuracy of millimeter wave measurements has been discussed previously[6].

The data acquisition process is initiated by the first frequency marker after the raw markers have been converted into square wave pulses. The markers are derived in the conventional way from the beat frequency between the klystron fundamental frequency and a harmonic of the frequency standard output in a mixing crystal, as indicated in Figure 1. An adjustable gate before the trigger input suppresses the second marker and all spurious signals which might also trigger the data acquisition process. This unit has proved to make the adjustment of the sweep conditions much less difficult than was pre-

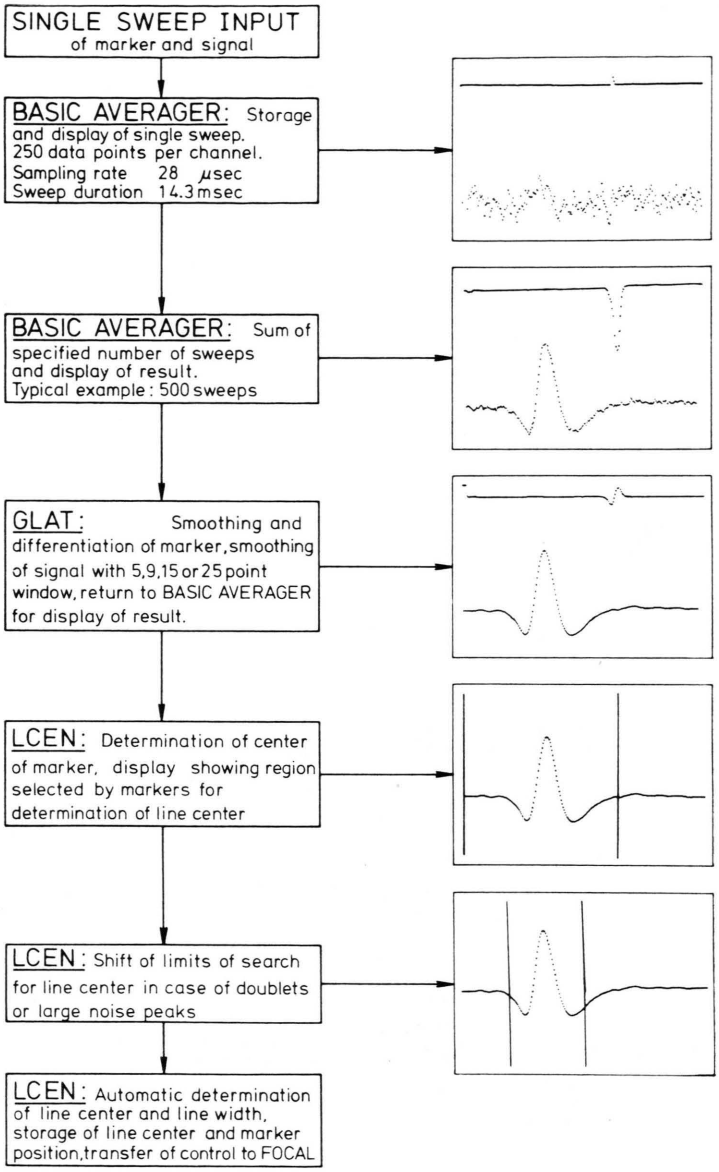


Fig. 2. Software aspects of the data acquisition system. BASIC AVERAGER, GLAT, LCEN and FOCAL are programs for successive steps in the measurement of a spectral line. The photographs to the right show the effect of each step on the data buffer as displayed on an oscilloscope.

viously the case. Finally, both markers and the absorption signal are multiplexed, digitized and accumulated by the computer.

Figure 2 shows the software aspects of the data acquisition and reduction system. The programs are called into core from the disk via the teletype at the discretion of the operator. Each step of the procedure is monitored on the display unit using the display routine in BASIC AVERAGER, which is called into the upper 4 K core storage and remains there during the entire procedure. Upon completion of averaging control is transferred to the program GLAT, which is called into the lower 4 K of core storage. This program smooths both the markers and the absorption signal and differentiates the markers according to the method of Savitzky and

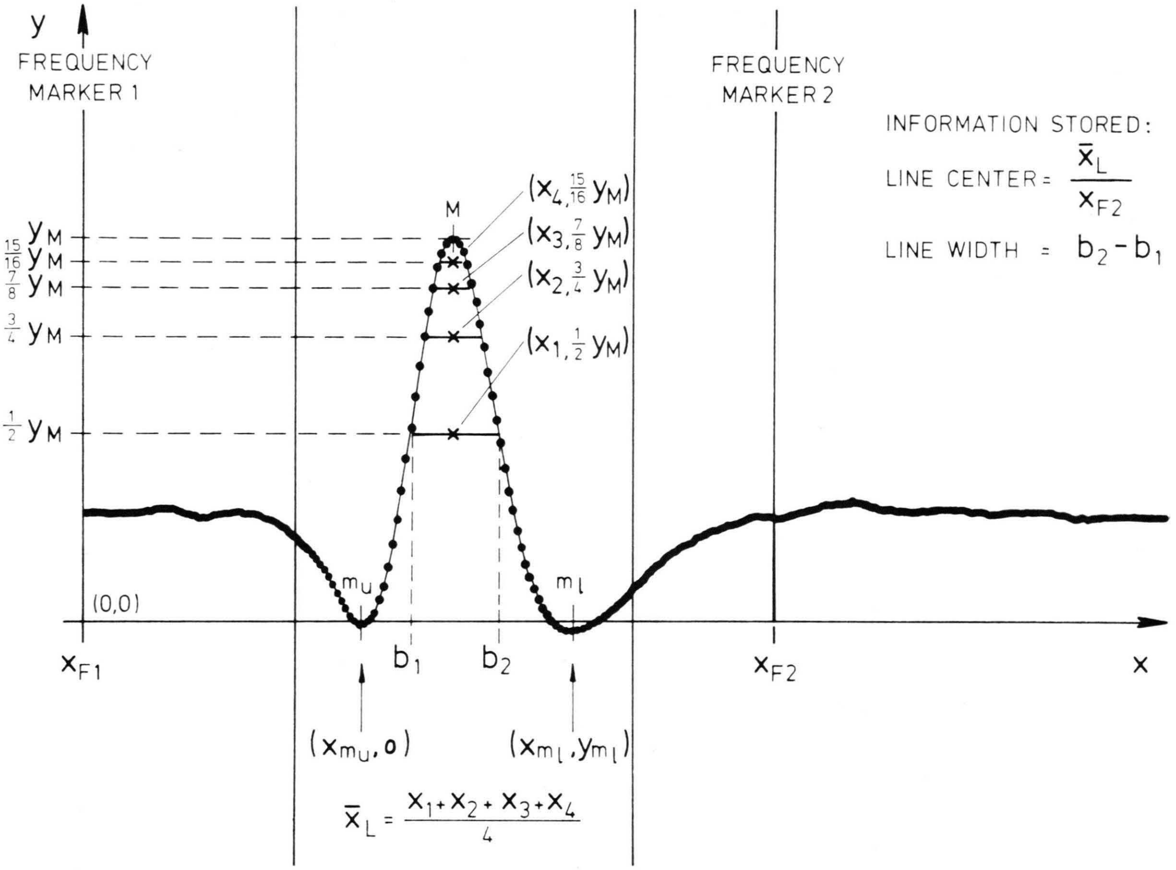


Fig. 3. Procedure used in automated determination of the center position of a millimeter wave spectral line by linear interpolation between frequency markers.

Golay[9], which does not alter either the line shape or the line width. The averaged marker, in contrast to the absorption signal, has usually a gaussian form, so that when the curve has been differentiated it is subsequently easy to determine the marker position by finding the point where the curve crosses the baseline. 24-bit arithmetic is used in the programs BASIC AVERAGER and GLAT. The smoothed data are returned to the data buffer in BASIC AVERAGER, where they may be inspected in the display as in Figure 2. GLAT is then replaced in the lower 4 K of core by LCEN. This program first determines and stores automatically the position of the center of the differentiated marker, interpolated between the channel positions along the frequency axis, and then displays the signal and the two marker positions. Only the region between the display markers will be searched for the line center, and the operator may shift each of them, as indicated in Fig. 2, to frame each line in the case of multiple lines. The line position is then located as shown in Fig. 3 in the following steps, using 24-bit arithmetic:

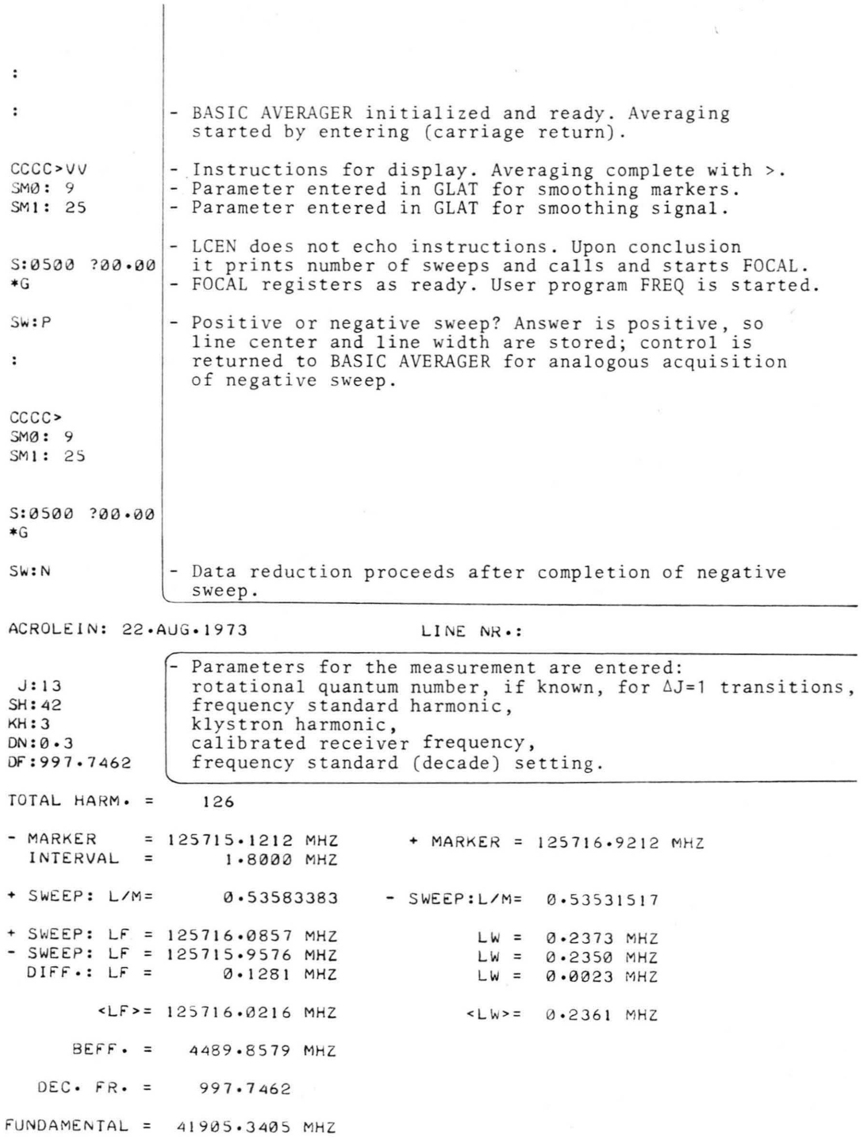
1) The absolute maximum between the adjustable display markers is found.

2) The absolute minima to the left and to the right of the maximum but within the display markers are found.

3) The upper minimum and the first frequency marker suffice to fix the coordinate system.

4) The height of the maximum, y_M, is divided by 2.

5) The endpoints of the chords corresponding to the four specified fractions of y_M are found by linearly interpolating between the coordinates of the pairs of points adjacent to the chords. Using the interpolated coordinates, the midpoint x_i of each chord is then taken as indicated in Figure 3. $\bar{x}_L$ is the average of these four midpoints.



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:

:                    - BASIC AVERAGER initialized and ready. Averaging
                       started by entering (carriage return).

CCCC>VV              - Instructions for display. Averaging complete with >.
SM0: 9               - Parameter entered in GLAT for smoothing markers.
SM1: 25              - Parameter entered in GLAT for smoothing signal.

                     - LCEN does not echo instructions. Upon conclusion
S:0500  ?00.00         it prints number of sweeps and calls and starts FOCAL.
*G                   - FOCAL registers as ready. User program FREQ is started.

SW:P                 - Positive or negative sweep? Answer is positive, so
                       line center and line width are stored; control is
:                      returned to BASIC AVERAGER for analogous acquisition
                       of negative sweep.

CCCC>
SM0: 9
SM1: 25


S:0500  ?00.00
*G

SW:N                 - Data reduction proceeds after completion of negative
                       sweep.

ACROLEIN: 22.AUG.1973                   LINE NR.:

                     - Parameters for the measurement are entered:
 J:13                  rotational quantum number, if known, for ΔJ=1 transitions,
SH:42                  frequency standard harmonic,
KH:3                   klystron harmonic,
DN:0.3                 calibrated receiver frequency,
DF:997.7462            frequency standard (decade) setting.

TOTAL HARM. =     126

- MARKER     = 125715.1212 MHZ      + MARKER = 125716.9212 MHZ
  INTERVAL   =       1.8000 MHZ

+ SWEEP: L/M=       0.53583383    - SWEEP:L/M=  0.53531517

+ SWEEP: LF  = 125716.0857 MHZ              LW =  0.2373 MHZ
- SWEEP: LF  = 125715.9576 MHZ              LW =  0.2350 MHZ
  DIFF.: LF  =       0.1281 MHZ             LW =  0.0023 MHZ

         <LF>= 125716.0216 MHZ            <LW>=  0.2361 MHZ

       BEFF. =   4489.8579 MHZ

    DEC. FR. =    997.7462

FUNDAMENTAL =  41905.3405 MHZ
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Fig. 4. Actual teletype record of a line measurement with explanatory comments in the boxed areas. Final result is the average of the measurements for both positive and negative sweep.

6) The information finally stored by the computer is the line center position relative to the frequency marker interval, and the effective line width, which corresponds to a constant fraction of the conventionally defined line width.

In the last step control is automatically transferred to FOCAL, an on-line compiler language, which replaces LCEN in core and is used to complete the primary data reduction.

A FOCAL user program to fetch the stored line center information and accept additional parameters from the teletype is also stored on the disk and is automatically called with FOCAL. It calculates the actual frequency of the line, and any other information desired. This compiler language program may be changed daily according to the molecule or the wishes of the operator. In Fig. 4 an actual teletype printout is shown. Such a printout constitutes a complete record of a line measurement including positive and negative sweeps. Occasionally a photograph or a plot of the signal on an X-Y recorder is made to show doublets or groups of lines.

The procedure described above for determining the line frequency of an averaged absorption signal was developed to fulfill as well as possible the following requirements:

1) The computer facility is limited to the configuration given above; 24-bit arithmetic may be used in assembler language programs and ten decimal digits (48 bits including exponent) in FOCAL.

2) Total expenditure of programmer time should not be excessive.

3) The operator need not be familiar with the computer or the assembler language, but should be able to change the form of the final printout and have control over the procedure.

4) Waiting for long calculations by the computer should be avoided.

5) The line positions must be reproducible to within at least a twentieth of the line width and within a fraction of the marker width.

6) The determination of the line center should use as much as possible of the total information content of the signal.

7) Since the shapes of absorption lines detected with the video technique vary and are asymmetric, the procedure must be more or less independent of line shape function. The asymmetry is consistent when the adjustment is correct, so that it can be eliminated in the final result by evaluating a positive and a negative sweep of each line and averaging the two values of the line position. This requires that sample pressure and electronic spectrometer adjustment remain constant during the data acquisition phase of both sweeps.

8) The highest point resolution we can obtain with the present averaging software is approximately 70 data points per line.

9) The signal-to-noise ratio is highly variable, and may be poor even after averaging.

We were able to satisfy the first three of these requirements by using the Digital Equipment Corporation programs BASIC AVERAGER and FOCAL unchanged except in the manner of storing them. The remaining programs were written in PDP-8/I assembler language except for the FOCAL user program which produces the final printout. The length of each program was not critical, since we use the disk and the interrupt facility to call each successive program with a one-letter instruction.

In the last year, while the final touches were being put on the system, we have measured nearly 1000 absorption lines with the resulting routine procedure. The advantages of the system may be summarized as follows:

1) Turn around time for measuring an absorption line with 500 sweeps for both positive and negative sweep is about 3 minutes.

2) Immediate calculation of the actual line frequency is made so that the assignment of new spectra becomes more efficient.

3) Human error is eliminated in judging the position of line centers and in repeated transfers of parameters.

4) For constant sample pressure the reproducibility of line positions is ± 5 kHz for strong lines up to 300 GHz, which corresponds to about 1/50 of the line width.

The first three factors give a considerable improvement in efficiency in comparison with earlier millimeter wave measurement techniques, including the first stage in the development of this system[6]. The improvement in reproducibility over our earlier results is a factor of 2 or more.

III. The Millimeter Wave Spectrum of DCNO

A) Sample Preparation

Several samples of DCNO were prepared according to the method described in Reference[3]. Some improvement in the yield could be obtained by inverting the decomposition step, that is, by dropping, the sodium fulminate solution into precooled (-5 °C to 0 °C) sulfuric acid through which a strong stream of nitrogen was blown. In a further attempt to increase the yield and the degree of deuteration, we tried omitting the drying tube filled with P_2O_5 which was used for HCNO preparations. Such "wet" samples did indeed have a higher proportion of D to H ($\geqq 90\%$ deuteration), but because of the presence of D_2O in the sample, decomposition and polymerization were considerably faster than in "dry" samples, even at the low pressure adequate for millimeter wave spectroscopy. "Wet" samples have a half-life of 5 to 10 minutes in the absorption cell at $5 \cdot 10^{-3}$ torr with a surprisingly high yield of DNCO. With the decay product we were able to

Table 1. Observed and calculated frequencies in MHz of rotational transitions in the ground state of $D^{12}C^{14}N^{16}O$.

$J+1 \leftarrow J$	Rigid rotor frequencies	Centrifugal distortion contribution	Calculated frequencies [a]	Observed frequencies [b]	obs. − calc.
$1 \leftarrow 0$	20584.9666	−0.0142	20584.9524	20585.00 [c]	0.0476
$2 \leftarrow 1$	41169.9331	−0.1133	41169.8202	41169.825	0.0048
$3 \leftarrow 2$	61754.8999	−0.3825	61754.5178	61754.540	0.0221
$4 \leftarrow 3$	82339.8662	−0.9067	82338.9604	82338.9582	−0.0023
$5 \leftarrow 4$	102924.8330	−1.7709	102923.0630	102923.0715	0.0085
$6 \leftarrow 5$	123509.8000	−3.0602	123506.7406	123506.7341	−0.0065
$7 \leftarrow 6$	144094.7660	−4.8594	144089.9081	144089.9136	0.0055
$8 \leftarrow 7$	164679.7320	−7.2537	164672.4806	164672.4757	−0.0049
$9 \leftarrow 8$	185264.6990	−10.3280	185254.3731	185254.3744	0.0013
$10 \leftarrow 9$	205849.6660	−14.1674	205835.5005	205835.4991	−0.0014
$11 \leftarrow 10$	226434.6330	−18.8568	226415.7779	226415.7775	−0.0004
$12 \leftarrow 11$	247019.6000	−24.4813	246995.1202	246995.1071	−0.0131
$14 \leftarrow 13$	288189.5310	−38.8754	288150.6560	288150.7607 [d]	0.1047
$16 \leftarrow 15$	329359.4650	−58.0297	329301.4389	329301.4448	0.0059

[a] Calculated frequencies were obtained using the constants in Table 5. The standard deviation of the fit is 9 kHz.
[b] The estimated experimental error for the millimeter wave lines is ±10 kHz.
[c] From Ref. [1]. Not included in least squares fit.
[d] Not included in least squares fit.

measure several transitions of the spectrum of DNCO with all K components. "Dry" samples allowed 30 to 40 minutes measuring time before the intensity was seriously reduced by decay or hydrogen exchange.

B) Measured Absorption Frequencies

The observed ground state lines, listed in Table 1, were fitted to the frequency expression

$$\nu = 2(J+1)B_v - 4(J+1)^3 D_v \,, \tag{1}$$

and the rotational constant B_0 and the centrifugal distortion constant D_0 are given in Table 5.

The frequencies of the two components of rotational transitions in a singly excited bending mode of a linear molecule are given by

$$\nu_{\pm} = 2(J+1)(B_v + 2D_v) - 4(J+1)^3 D_v \pm \tfrac{1}{2}[2(J+1)\, q_t^{(0)} - 4(J+1)^3\, q_t^{(1)}] \tag{2}$$

in which $q_t^{(0)}$ is the l-type doubling constant for the t-th mode and $q_t^{(1)}$ describes the J-dependence of the l-type doubling. We have determined the constants B_v and D_v for the states $v_5 = 1$ and $v_4 = 1$ by fitting the sum of the two components for each J as shown in Tables 2 and 3, and the constants $q_t^{(0)}$ and $q_t^{(1)}$ by fitting the difference of the two components as shown in Table 4. The constants obtained from the least squares procedure are given in Table 5. In addition we have listed in Table 6 the constants obtained by fitting the individual components of the l-type doublet transitions. For both $v_4 = 1$ and $v_5 = 1$, the more accurate values obtained from the direct l-type doubling transitions [3] for $q_t^{(0)}$

Table 2. Observed frequencies and deviations (obs. − calc.) in MHz of rotational transitions in the 0001^10^0 vibrational state of $D^{12}C^{14}N^{16}O$.

$J+1 \leftarrow J$	Observed doublet [b]		Center of doublet	
	$(0001^10)_c$	$(0001^10)_d$	observed	obs. − calc. [a]
$2 \leftarrow 1$	41188.125	41259.774	41223.9495	0.0055
$3 \leftarrow 2$	61781.961	61889.413	61835.6870	−0.0105
$4 \leftarrow 3$	82375.5585	82518.7823	82447.1704	−0.0185
$5 \leftarrow 4$	102968.8137	103147.8735	103058.3436	0.0128
$6 \leftarrow 5$	123561.6039	123776.4788	123669.0414	0.0056
$7 \leftarrow 6$	144153.8868	144404.5445	144279.2156	−0.0009
$8 \leftarrow 7$	164745.5691	165032.0019	164888.7855	0.0000
$9 \leftarrow 8$	185336.5540	185658.7535	185497.6537	0.0017
$10 \leftarrow 9$	205926.7614	206284.7201	206105.7408	0.0019
$11 \leftarrow 10$	226516.1272	226909.7830	226712.9551	0.0065
$12 \leftarrow 11$	247104.4939	247533.8883	247319.1911	−0.0060

[a] Calculated frequencies were obtained using the constants in Table 5. The standard deviation of the fit is 9 kHz.
[b] The estimated experimental errors for the millimeter wave lines is ±10 kHz.

Table 3. Observed frequencies and deviations (obs. − calc.) in MHz of rotational transitions in the $0000^0 1^1$ vibrational state of $D^{12}C^{14}N^{16}O$.

$J+1 \leftarrow J$	Observed doublet [b] $(0000^0 1^1)_c$	$(0000^0 1^1)_d$	Center of doublet observed	obs. − calc. [a]
$2 \leftarrow 1$	41278.385	41430.727	41354.556	0.0052
$3 \leftarrow 2$	61917.354	62145.863	62031.6085	−0.0004
$4 \leftarrow 3$	82556.0672	82860.7411	82708.4042	−0.0022
$5 \leftarrow 4$	103194.4766	103575.2220	103384.8493	−0.0069
$6 \leftarrow 5$	123832.4797	124289.2911	124060.8854	0.0138
$7 \leftarrow 6$	144469.9449	145002.7810	144736.3630	−0.0025
$8 \leftarrow 7$	165106.8506	165715.6397	165411.2451	−0.0061
$9 \leftarrow 8$	185743.0680	186427.8052	186085.4366	−0.0050
$10 \leftarrow 9$	206378.5571	207139.1575	206758.8573	0.0073
$11 \leftarrow 10$	227013.1998	227849.5803	227431.3901	0.0007
$12 \leftarrow 11$	247646.9444	248558.9983	248102.9714	−0.0015
$14 \leftarrow 13$	288911.7860 [c]			

[a] Calculated frequencies were obtained using the constants in Table 5. The standard deviation of the fit is 7 kHz.

[b] The estimated experimental error for the millimeter wave lines is ±10 kHz.

[c] Not included in the least squares fits.

Table 4. Observed frequencies and deviations (obs. − calc.) in MHz of splittings between the rotational transitions in the $0000^0 1^1$ and $0001^1 0^0$ vibrational states of $D^{12}C^{14}N^{16}O$.

$J+1 \leftarrow J$	Doublet separation for $0000^0 1^1$ observed	obs. − calc. [a]	Doublet separation for $0001^1 0^0$ observed	obs. − calc. [a]
$2 \leftarrow 1$	152.342	−0.0076	71.649	0.0112
$3 \leftarrow 2$	228.509	0.0027	107.452	−0.0008
$4 \leftarrow 3$	304.6739	0.0327	143.2238	−0.0394
$5 \leftarrow 4$	380.7454	−0.0016	179.0598	−0.0076
$6 \leftarrow 5$	456.8114	−0.0052	214.8749	0.0111
$7 \leftarrow 6$	532.8361	−0.0064	250.6577	0.0066
$8 \leftarrow 7$	608.7891	−0.0286	286.4328	0.0053
$9 \leftarrow 8$	684.7372	0.0024	322.1995	0.0080
$10 \leftarrow 9$	760.6004	0.0138	357.9587	0.0170
$11 \leftarrow 10$	836.3805	0.0148	393.6558	−0.0206
$12 \leftarrow 11$	912.0539	−0.0111	429.3944	0.0003

[a] Calculated separations were obtained using the constants in Table 5. The standard deviation of both fits is 17 kHz.

Table 5. Molecular constants of $D^{12}C^{14}N^{16}O$ obtained from the centrifugal distortion analysis [a].

Vibrational state $v_1\ v_2\ v_3\ v_4^l\ v_5^l$	B_v/MHz	D_v/kHz	$q_t^{(0)}$/MHz	$q_t^{(1)}$/kHz
$0\ 0\ 0\ 0^0\ 0^0$	10292.48340 (31)	3.5418 (10)		
$0\ 0\ 0\ 0\ 1^1$	10338.65942 (32)	3.6208 (16)	38.08983 (84)	.3025 (41)
$0\ 0\ 0\ 1^1\ 0^0$	10306.00780 (45)	3.6409 (22)	17.90995 (86)	.0644 (42)

[a] Errors quoted are standard errors.

Table 6. Rotational constants of the individual components of the rotational l-type doublet transitions [a].

Vibrational state $v_1\ v_2\ v_3\ v_4^l\ v_5^l$	B_v/MHz	D_v/kHz	Standard deviation of fit/kHz
$(0\ 0\ 0\ 0^0\ 1^1)_c$	10319.61481 (49)	3.4696 (24)	10
$(0\ 0\ 0\ 0^0\ 1^1)_d$	10357.70403 (56)	3.7720 (28)	11
$(0\ 0\ 0\ 1^1\ 0^0)_c$	10297.05293 (46)	3.6087 (23)	9
$(0\ 0\ 0\ 1^1\ 0^0)_d$	10314.96276 (75)	3.6731 (37)	15

[a] Errors quoted are standard errors.

and $q_t^{(1)}$ are within three times the standard error of the constants obtained from the present data.

IV. Discussion

The ground state constants shift upon deuteration as expected. Although the values of α_t and q_t for the states ν_4 and ν_5 were reported earlier [3], the recent assignment of the vibrational spectrum of both the normal and deuterated species of fulminic acid allows us to update the discussion of these constants.

The value of α_5 shifts strongly upon deuteration, going from −30.1 MHz in HCNO to −46.2 MHz in DCNO. This shift can now be understood as a result of the fact that ν_5 is a large-amplitude HCN bending mode, the energy of which drops strongly upon deuteration from 224 cm^{-1} to 163 cm^{-1} (see Ref. [7]) so that the α_5 value is expected to increase in magnitude. The value of α_5 for HCNO is well reproduced by calculations using the Hougen, Bunker, Johns Hamiltonian extended to four-atomic molecules by Stone [10]. The value of α_4, on the other hand, shifts only from -14.4 MHz in HCNO to -13.5 MHz in DCNO. This small decrease is of the order of magnitude expected due to the smaller rotational constant, and indicates very little shift in the vibrational frequency of ν_4, which is 538 cm^{-1} in HCNO [7].

The dependence of $q_t^{(0)}$ upon deuteration cannot be explained so simply. In the harmonic approximation $q_t^{(0)}$ is given by

$$q_t^{(0)} = \frac{B_e^2}{\omega_t} 2 \left[1 + 4 \sum_i \left\{ (\xi_{it}^x)^2 \frac{\omega_t^2}{\omega_i^2 - \omega_t^2} \right\} \right] \quad (3)$$

which can be approximated by the empirical relation

$$q_t^{(0)} = (B_e^2/\nu_t)\,\mathbf{f} \quad (4)$$

where **f** falls between 1.9 and 2.9 for linear molecules so far measured [1]. The values of **f** obtained for HCNO and DCNO are

	H	D
ν_4	2.87	–
ν_5	1.77	1.76

A glance at Eq. (3) shows that for the lowest bending mode, ν_5, the summation must be positive, so that **f** should be greater than 2.0. Since this is not the case, we have further evidence that the ν_5 mode is strongly anharmonic. For HCNO the $q_5^{(0)}$ value has been calculated by Stone [10] using the rigid-bender molecular Hamiltonian and is in agreement with the experimental results.

Since we have found that HCNO can best be described as a quasilinear molecule, we can correlate $q_5^{(0)}$ with the difference of rotational constants $(C-B)$ of an asymmetric rotor. Assuming the CNO chain to be rigid, we calculated the HCN (DCN) angle which would give the observed value of $(C-B)$. For HCNO we find 158° and for DCNO 162° for the average value of the HCN (DCN) angle. These values are compatible with those found by roughly fitting the vibrational levels to a potential function with a barrier, which range between 155° and 170° (see [7]).

There is no anomalous centrifugal distortion contribution to the *l*-type doubling of either ν_4 or ν_5 in DCNO. The anomalous effects found for ν_4 in HCNO may be explained by an accidental Coriolis resonance which will be discussed in a separate publication [11].

Acknowledgment

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