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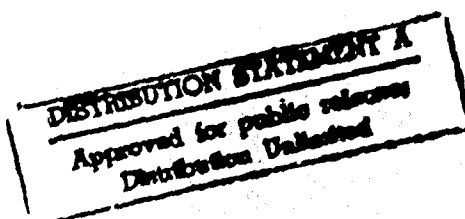
Line Intensities and Self-Broadening Coefficients
of $^{12}\text{C}^{16}\text{O}_2$ and $^{13}\text{C}^{16}\text{O}_2$ Lines in the Laser Band Region

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The intensities of $^{12}\text{C}^{16}\text{O}_2$ and $^{13}\text{C}^{16}\text{O}_2$ lines have been measured in the laser band region (around $10\mu\text{m}$), using Fourier transform spectra. For each studied band the square of the transition dipole moment and Herman-Wallis coefficients have been determined. The band intensities deduced from these results are in good agreement with those obtained by the Direct Numerical Diagonalization calculations. In addition the self broadening coefficients have been measured.			
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SCIENTIFIC REPORT

Line Intensities and Self-Broadening Coefficients of $^{12}\text{C}^{16}\text{O}_2$ and $^{13}\text{C}^{16}\text{O}_2$ Lines in the Laser Band Region

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This report is divided into two parts: the first part is devoted to the methodology of the measurements and to the $^{12}\text{C}^{16}\text{O}_2$ molecule, and the second part to the $^{13}\text{C}^{16}\text{O}_2$ isotopic species.

PART I

Line intensities and self-broadening coefficients of $^{12}\text{C}^{16}\text{O}_2$ lines in the laser band region. Methodology of the measurements

SUMMARY

The intensities of $^{12}\text{C}^{16}\text{O}_2$ lines have been measured in the four bands centered at 927.156, 960.959, 1063.735, and 1071.542 cm^{-1} , using Fourier transform spectra. The square of the transition dipole moment and Herman-Wallis coefficients have been determined; the band intensities deduced from these results are in good agreement with those obtained by the Direct Numerical Diagonalization calculations. In addition, the self-broadening coefficients of 90 lines have been measured in the two strongest bands.

I. INTRODUCTION

In its laser band region, the main isotopic species of carbon dioxide gives rise mainly to four parallel hot bands around $10\mu\text{m}$. Among them, the strongest are the 00011-10001 and 00011-10002 bands centered respectively at 960.959 and 1063.735 cm^{-1} , the other two being the 01111-11101 and 01111-11102 weak bands centered respectively at 927.156 and 1071.542 cm^{-1} . The last published experimental results concerning these bands are those of Abubakar and Shaw (see Ref. (1) and its bibliography where the references of earlier works can be found). The last intensity calculations are those of Wattson and Rothman (2), who used a Direct Numerical Diagonalization method (hereafter denoted as DND). At the present time, the data available through the 1986 version of the HITRAN database (3) are currently used for various radiative transfer studies.

We present here the results of systematic measurements of line intensities in the four above-mentioned bands. High resolution Fourier transform spectra (unapodized FWHM = $2.7 \times 10^{-3}\text{ cm}^{-1}$) have been used to retrieve accurate absolute line and band intensities, and it appeared that our results compare better with the last DND calculated values (2) than with the 1986 HITRAN values (3). The self-broadening coefficients of 90 lines pertaining to the two strongest bands were also measured: they do not reveal any vibrational dependence.

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II. EXPERIMENTAL DETAILS

The intensities and self-broadening coefficients measurements were performed on five spectra recorded with the Fourier transform spectrometer of the Laboratoire de Physique Moléculaire et Applications, at the Université Paris-Sud. The experimental conditions are summarized in Table I.

The length of the absorption path inside the White-type cell is very well known. The pressure has been measured with an uncertainty of 0.1 Torr. So, the uncertainties on these two quantities ($\approx 0.1\%$ on the absorption path and $\approx 0.2\%$ on the gas pressure) have very small effects on the retrieved line parameters. On the contrary, since we are studying hot bands, it is necessary to know the temperature with a good accuracy. The temperature was measured in three places: in the room, on the cell walls, and inside the cell. The equality of the three measured values has shown that a thermal equilibrium had been reached during the recording of each interferogram. However, as a recording takes around ten hours, small variations of the temperature occur. The values of the temperatures reported in Table I are average values which define the temperature of our measurements with a maximum uncertainty of ± 1 K.

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III. METHOD OF MEASUREMENTS

III.1. Treatment of the channeled spectra

In the studied spectral region, fringes, caused by multiple optical reflections on the opposite sides of the beam splitter, appear on the spectra. Figures 1 and 2 show portions of typical channeled spectra. The presence of a channel of this type is a source of difficulties in the treatment of the spectra, since it has been proved that it could hardly affect the line positions and intensities (4, 5). In recent works (see, e.g., Refs. (6, 7)), a channel observed on spectra has been taken into account in the treatment. However, we have to point out the fact that the fringes we are dealing with in this work come from multiple reflections inside the interferometer; they have not to be confused with fringes due to multiple reflections on the filter or on the windows of the apparatus. In the following, we will discuss how we have removed the channel from our spectra, without introducing additional errors.

In Ref. (5), it has been shown that the second reflection on the sides of the beam splitter gives rise to two secondary interferograms in addition to the main interferogram $I(\Delta)$, and that the actual recorded interferogram is

$$I'(\Delta) = I(\Delta) + \gamma_1 I(\Delta - \delta) + \gamma_2 I(\Delta + \delta), \quad (1)$$

where Δ is the path difference between the fixed and moving mirrors, and δ the path difference between the opposite sides of the beam splitter (γ_1 and γ_2 are related to the reflection and transmission coefficients of the sides of the beam splitter). From Eq. (1), one can deduce (5) the expression of the transmission $T(\sigma)$, resulting from an isolated absorption line of profile $g(\sigma - \sigma_0)$ centered at σ_0 :

$$\begin{aligned} T(\sigma) = & T_b(\sigma) \{ [1 - g(\sigma - \sigma_0)] * f(\sigma \Delta_{\max}) \\ & + 2 \gamma_2 \cos(2\pi\sigma\delta) * f(\sigma \Delta_{\max}) \\ & - [g(\sigma - \sigma_0) (\gamma_1 + \gamma_2) \cos(2\pi\sigma\delta)] * f(\sigma \Delta_{\max}) \} \end{aligned}$$

$$- [g(\sigma - \sigma_0) (\gamma_1 - \gamma_2) \sin(2\pi\sigma\delta)] * h(\sigma\Delta_{\max})\}, \quad (2)$$

where the symbol $*$ represents a convolution product. $T_b(\sigma)$ is the low resolution envelope: since its variation is very weak along a line, it has not be included in the convolution product, so in the following, in order to simplify the notation, $T(\sigma)$ will represent the ratio $T(\sigma)/T_b(\sigma)$. $f(\sigma\Delta_{\max})$ and $h(\sigma\Delta_{\max})$ are the symmetrical and antisymmetrical apparatus functions respectively (8):

$$f(\sigma\Delta_{\max}) = 2 \Delta_{\max} \sin(2\pi\sigma\Delta_{\max}) / 2\pi\sigma\Delta_{\max}, \quad (3)$$

$$\text{and } h(\sigma\Delta_{\max}) = 2 \Delta_{\max} [1 - \cos(2\pi\sigma\Delta_{\max})] / 2\pi\sigma\Delta_{\max}, \quad (4)$$

$\Delta_{\max}$ being the maximum path difference.

Equation (2) is the complete expression of a channeled spectrum. The first term between braces is the usual unchanneled spectrum. The second term represents the sine channel observable on the continuous background (note that because of small variations of the beam splitter indices with the wavenumber, the amplitude and the period of the experimental channel can change very slightly along the spectrum). The second and third terms of Eq. (2) perturb the line depth and can cause errors in line intensity measurements if they are not taken into account in the analysis. The fourth term leads to an asymmetry in the line shape; it can cause noticeable errors in line position measurements (8).

In absence of absorbing gas, only the second term and the constant in the first term of Eq. (2) are different from zero. Since in usual experimental conditions the period of the channel is much larger than the resolution limit, one can write the expression of the channel in absence of absorption as $T_0(\sigma)$

$$T_0(\sigma) = 1 + 2 \gamma_2 \cos(2\pi\sigma\delta). \quad (5)$$

In the vicinity of each studied line, $T_0(\sigma)$ can be obtained fitting the continuous background by Eq. (5) on wide domains on each side of the studied line, where the influence of this line and of the neighboring ones is negligible ($\leq 0.1\%$). Moreover, Eq. (5)

shows that ratioing the channeled spectrum (Eq. 2) against an empty cell background exhibiting the same channel (Eq. 5) puts the channel out of sight on the resulting plotted spectrum, but is not sufficient to avoid errors in line positions and intensities, since only the second term of Eq. 2 has been removed.

A similar problem occurs in the zero transmission determination from saturated lines. Indeed, on the top of such a line, considering that $g(\sigma - \sigma_0)$ remains constant (equal to 1) on a spectral domain much larger than the resolution limit, one can write the expression of the transmission as $T_s(\sigma)$:

$$T_s(\sigma_0) = (\gamma_2 - \gamma_1) \cos(2\pi\sigma_0\delta). \quad (6)$$

This expression shows that the transmission $T_s(\sigma_0)$ around the center of a saturated line depends on the position of this line with respect to the channel, as can be seen on Fig. 2. Consequently, spectra with saturated lines can be advantageously used to obtain the variation $T_s(\sigma)$ of the true zero transmission level with the wavenumber. Practically, wide sets of broad saturated lines, having various positions with respect to the channel, were used to obtain $T_s(\sigma)$ from the experimental data through a least squares fit. Thus, we could check that:

- first, $T_s(\sigma)$ is actually well described by a sine function;
- and second, $T_0(\sigma)$ and $T_s(\sigma)$ have the same phase, according to the usual values (5) of γ_1 and γ_2 ; also, the ratio of their amplitudes is constant along each spectrum.

All this suggests the following procedure to treat correctly a channeled spectrum. Equations (2,5,6) lead to:

$$t(\sigma) = [T(\sigma) - T_s(\sigma)] / [T_0(\sigma) - T_s(\sigma)] \quad (7)$$

$$\neq [1 - g(\sigma - \sigma_0)] * [f(\sigma\Delta_{\max}) + \rho h(\sigma\Delta_{\max})], \quad (8)$$

$$\text{with } \rho = [(\gamma_1 - \gamma_2) \sin(2\pi\sigma_0\delta)] / [1 + (\gamma_1 + \gamma_2) \cos(2\pi\sigma_0\delta)]. \quad (9)$$

Since the values observed for $|\rho|$ are very small (typically, less than 0.1), Eq. (1) can formally be rewritten as:

$$t(\sigma) = [1 - q(\sigma - \sigma_0)] * q(\sigma - \sigma_0) \quad (10)$$

with

$$q(\sigma \Delta_{\max}) = [\cos \phi f(\sigma \Delta_{\max}) + \sin \phi h(\sigma \Delta_{\max})], \quad (11)$$

$\sin \phi = \rho$, and $\cos \phi \neq 1$.

$t(\sigma)$ represents the convolution of the absorption line by an asymmetrical apparatus function $q(\sigma \Delta_{\max})$; the spectrum is correctly dischanneled, contrary to that happens when one performs the ratio $T(\sigma)/T_0(\sigma)$. For each line the effective apparatus function $q(\sigma \Delta_{\max})$ depends on a parameter ϕ ; this parameter plays a similar role than the parameter describing a phase error (8).

Practically, $T_0(\sigma)$ and $T_s(\sigma)$ are measured on the spectra as explained above, and the values of $t(\sigma)$ are obtained using Eq. (7) at each primary point of the spectrum.

III.2. The apparatus function

As said above, a correct treatment of $t(\sigma)$ needs the use of an asymmetrical apparatus function. The parameter ϕ in $q(\sigma \Delta_{\max})$ is adjusted for each line according to its position with respect to the channel, in order to reach the best fit. It was checked in Ref. (8) that it is necessary to take into account the effect of the parameter ϕ , to avoid relative errors of few percents in the intensity and line width measurements.

Furthermore, to obtain accurate line intensities and widths, it is advisable to take into account the slight apodization due to the trough-put. In a previous work (9), we had established an analytical expression for the symmetrical apodized apparatus function. This expression was used in Eq. (11) in place of $f(\sigma \Delta_{\max})$.

III.3. The fitting procedure

To obtain the line parameters, a spectrum, computed using Eq. (10), is adjusted, for each primary point, to the experimental

values of $t(\sigma)$ (determined as explained in Section III.1). In Eq. (10), the apparatus function described in Section III.2 was used. $g(\sigma-\sigma_0)$ is the absorption line shape under infinite resolution:

$$g(\sigma-\sigma_0) = \exp[-S^\circ PL (1/\gamma^D) (\text{Log}2/\pi)^{1/2} k(x,y)], \quad (12)$$

with S° = line intensity,

P = pressure of the absorbing gas,

L = length of the absorbing path,

γ^D = Doppler half-width,

γ^L = Lorentz half-width,

$x = (\text{Log}2)^{1/2} (\sigma-\sigma_0) / \gamma^D$,

$y = (\text{Log}2)^{1/2} \gamma^L / \gamma^D$,

and where $k(x,y)$ is the reduced Voigt profile calculated with the aid of the Gautschi's algorithm (10).

The intensity of some lines are missing since it was impossible to fit the channel in their vicinity, because of the presence of neighboring lines.

IV. DATA REDUCTION AND DISCUSSION OF THE RESULTS

IV.1. Line intensities

Using the method detailed in the previous section, we have measured more than 160 line intensities in the laser bands region of $^{12}\text{C}^{16}\text{O}_2$. The five spectra (Table I) have been used, and we checked that the lines which could be measured simultaneously in different spectra gave results in good agreement (discrepancy smaller than 2 %). Moreover, no systematic discrepancy appeared between the sets of line intensities deduced from different spectra.

Our results are reported in Tables II-V according to the bands; the intensities have been converted to cm/mol-unit at the reference temperature of the HITRAN database, i.e., 296 K. The uncertainty on these intensities will be discussed now. The treat-

ment of the channel avoid large errors on the line parameters determination, but it decreases slightly the signal to noise ratio. The residuals of the fits are mainly due to the noise. On the average, the statistical relative uncertainties on the obtained intensities is 2 %. An additional uncertainty comes from the uncertainty on the temperature (see Section II): several tests showed us that an error of 0.5 K on the temperature does not change the intensities by more than 2 %. On the whole, a maximum value of the uncertainty on our absolute line intensities is about 5 %.

For each band, we have derived the square of the transition dipole moment $|\mu|^2$, with respect to the running index m ($m = -J''$ in the P branch and $J''+1$ in the R branch, J'' being the rotational quantum number of the lower level). $|\mu|^2$ can be expressed as $|\mu|^2 = |\mu_0|^2 F(m)$, where $|\mu_0|^2$ is the vibrational dipole moment matrix element and $F(m)$ the F-factor including Herman-Wallis coefficients:

$$F(m) = [1 + A_1 m + A_2 J''(J''+1)]^2. \quad (13)$$

In addition, the relationship between the intensity of a transition between states i and f , S_{if} , and $|\mu|^2$ is given by:

$$S_{if}(T) = (8\pi^3/3hc) \sigma_{if} [1 - \exp(-c_2 \sigma_{if} / T)] (I_a/Q(T)) \times \exp(-c_2 E_i / T) L_{if} |\mu|^2 10^{-36}, \quad (14)$$

where σ_{if} is the frequency of the transition, c_2 is the second radiation constant (hc/k), I_a is the natural isotopic abundance, $Q(T)$ is the total internal partition sum, and E_i is the energy of the lower state. The units are cgs, except for $|\mu|$ which is in Debyes. The point to be noted is that in this definition the line intensities are functions of the temperature, T , and the isotopic abundance I_a , while $|\mu|^2$ is independent of these quantities. The transition moment constants obtained through a fit of the line intensities are reported in Table VI. Using Eq. (13), the line intensities have been calculated and compared with their experimental values (see Tables II-V). The agreement is good, as can also

be seen on Figs. 3-6.

From the usual relationship between the band intensity and the square of the transition dipole moment (2,11), we have calculated the intensities of the four studied bands. The obtained values are reported in Table VII together with the last published DND (2) and HITRAN (3) results. One can see that the DND calculated values agree better with our experimental results than with the 1986 HITRAN values. The slight discrepancies between our results and DND are smaller than our stated uncertainty (5%).

IV.2. Self-broadening coefficients

The fitting of the line profiles can give simultaneously the line intensities and the self-broadening coefficients. This was done for the two strongest bands, but this could not be possible for the two other bands because of the weakness of the lines. For these weak hot lines, the self-broadening coefficients were constrained to approximate values, close to those measured in other bands.

The measured self-broadening coefficients are listed in Table VIII and plotted on Fig. 7. The temperature is 294 ± 1 K, and the uncertainty on absolute values is 5%. Figure 7 shows that for the two concerned bands, no vibrational dependence appears.

V. CONCLUSION

Using Fourier transform spectra, systematic measurements of absolute line intensities have been performed in the $^{12}\text{C}^{16}\text{O}_2$ bands centered at 927.156, 960.959, 1063.735, and 1071.542 cm^{-1} , improving upon the previous experimental results. Also, self-broadening coefficients of lines belonging to the bands centered at 960.959 and 1063.735 cm^{-1} were measured. These results concerning the laser bands region of $^{12}\text{C}^{16}\text{O}_2$ will be useful for radiative transfer studies.

CAPTIONS OF THE TABLES

TABLE I. Experimental Conditions for the $^{12}\text{C}^{16}\text{O}_2$ spectra

TABLE II. Line Intensities for the 00011-10001 Band of $^{12}\text{C}^{16}\text{O}_2$

TABLE III. Line Intensities for the 00011-10002 Band of $^{12}\text{C}^{16}\text{O}_2$

TABLE IV. Line Intensities for the 01111-11101 Band of $^{12}\text{C}^{16}\text{O}_2$

TABLE V. Line Intensities for the 01111-11102 Band of $^{12}\text{C}^{16}\text{O}_2$

TABLE VI. Transition Moment Constants $|\mu_0|^2$, A_1 , and A_2 for $^{12}\text{C}^{16}\text{O}_2$

TABLE VII. Band Intensities S_v of the Studied Laser Bands of $^{12}\text{C}^{16}\text{O}_2$

TABLE VIII. Self-Broadening Coefficients Measured for Lines of the 00011-10001 and 00011-10002 Bands of $^{12}\text{C}^{16}\text{O}_2$, in $10^{-3} \text{ cm}^{-1} \cdot \text{atm}^{-1}$

TABLE I

Radius of the iris: 2.85 mm

Focal length of the collimator: 2000 mm

Signal to Noise Ratio: ≈ 150

Absorbing gas: 99.998 % minimum purity carbon dioxide in natural abundance
(i.e. 98.4 % of $^{12}\text{C}^{16}\text{O}_2$) purchased from Air Liquide

Spectrum number	Absorbing path (cm)	Total pressure (Torr)	Maximal path difference (cm)	Temperature (K)
1	5217	49.9	182.37	294.2
2	5217	49.9	184.01	293.8
3	2817	49.9	175.07	293.8
4	417	50.0	184.01	294.7
5	5217	100.0	184.01	294.2

TABLE II

Line	σ	S_{obs}	S_{cal}	%
P54	910.016	4.45	4.31	3.2
P52	912.231	6.32	6.25	1.2
P50	914.419	9.12	8.91	2.3
P44	920.829	22.91	23.31	-1.8
P40	924.974	40.89	40.58	0.7
P38	927.008	51.78	52.14	-0.7
P36	929.018	64.27	65.79	-2.4
P34	931.002	81.56	81.51	0.1
P32	932.961	96.03	99.09	-3.2
P30	934.894	115.00	118.19	-2.8
P28	936.804	132.40	138.20	-4.4
P24	940.548	175.80	177.42	-0.9
P22	942.383	196.40	194.53	1.0
P18	945.980	223.40	217.59	2.6
P16	947.742	228.20	220.88	3.2
P14	949.479	217.90	217.42	0.2
P12	951.192	205.40	206.37	-0.5
P10	952.881	190.50	187.64	1.5
P 8	954.545	156.80	161.27	-2.9
P 6	956.185	127.40	127.91	-0.4
P 4	957.801	87.51	88.85	-1.5
P 2	959.392	46.66	45.64	2.2
R 0	961.733	22.47	22.99	-2.3
R 2	963.263	67.10	68.08	-1.5
R 4	964.769	110.80	110.39	0.4
R 6	966.250	148.90	147.81	0.7
R 8	967.707	179.30	179.19	0.1
R10	969.140	204.20	203.26	0.5
R12	970.547	221.70	219.61	0.9
R14	971.930	229.80	228.10	0.7
R16	973.289	228.40	229.10	-0.3
R18	974.622	224.70	223.37	0.6
R20	975.930	213.70	212.32	0.6
R22	977.214	198.10	196.81	0.6
R24	978.472	180.40	178.29	1.2
R26	979.705	159.40	158.05	0.8
R28	980.913	139.00	137.15	1.3
R30	982.096	119.40	116.70	2.3
R32	983.252	95.90	97.35	-1.5
R34	984.383	77.45	79.71	-2.9
R36	985.488	65.55	64.05	2.3
R38	986.567	51.02	50.54	0.9
R40	987.620	38.85	39.17	-0.8
R42	988.647	29.64	29.81	-0.6
R44	989.646	22.46	22.31	0.7
R46	990.620	17.13	16.39	4.3
R48	991.566	11.60	11.84	-2.0

R50	992.485	8.28	8.41	-1.6
R52	993.376	5.80	5.88	-1.3
R54	994.240	3.98	4.04	-1.4
R56	995.077	2.76	2.73	1.1
R58	995.885	1.76	1.81	-3.0

Units are 10^{-26} cm/mol at 296 K in natural abundance. σ are the line positions in cm^{-1} . S_{obs} are the measured intensities and S_{calc} the intensities calculated using the transition moment constants listed in Table VI. % is the relative difference between these two values.

TABLE III

Line	σ	S_{obs}	S_{cal}	%
P60	1005.477	2.13	2.08	2.2
P56	1010.043	4.64	4.68	-0.8
P54	1023.189	6.86	6.92	-0.9
P52	1014.518	9.33	9.86	-5.7
P50	1016.721	13.97	14.05	-0.6
P48	1018.901	19.21	19.61	-2.1
P46	1021.057	25.56	26.64	-4.2
P44	1023.189	35.61	35.89	-0.8
P42	1025.298	47.71	47.53	0.4
P40	1027.382	65.61	61.88	5.7
P38	1029.442	76.48	79.12	-3.5
P36	1031.478	101.60	99.40	2.2
P34	1033.488	123.50	122.95	0.4
P32	1035.474	153.90	149.00	3.4
P30	1037.434	172.80	176.80	-2.3
P28	1039.369	214.80	206.15	4.0
P26	1041.279	242.80	235.55	3.0
P24	1043.163	269.30	263.76	2.1
P22	1045.022	294.90	288.82	2.1
P20	1046.854	303.40	308.90	-1.8
P18	1048.661	315.50	322.21	-2.1
P16	1050.441	319.40	326.99	-2.4
P14	1052.196	330.10	322.09	2.4
P12	1053.923	302.40	305.73	-1.1
P10	1055.625	287.20	278.35	3.1
P 8	1057.300	246.30	239.45	2.8
P 6	1058.949	189.10	190.28	-0.6
P 4	1060.571	131.40	132.26	-0.7
P 2	1062.166	66.51	69.04	-3.8
R 0	1064.509	33.96	34.49	-1.6
R 2	1066.037	104.90	102.48	2.3
R 4	1067.539	162.10	166.57	-2.8
R 6	1069.014	221.80	223.95	-1.0
R 8	1070.402	271.10	272.78	-0.6
R10	1071.884	311.20	311.32	-0.0
R12	1073.278	345.50	337.47	2.3
R16	1075.988	344.40	357.22	-3.7
R18	1077.302	354.70	349.62	1.4
R20	1078.591	319.50	334.45	-4.7
R22	1079.852	314.70	312.32	0.8
R26	1082.296	247.10	254.55	-3.0
R28	1083.479	223.20	222.93	0.1
R30	1084.635	192.00	191.25	0.4
R32	1085.766	160.70	161.01	-0.2
R36	1087.948	106.30	107.90	-1.5
R38	1089.001	86.34	86.05	0.3
R42	1091.030	52.25	49.08	6.1
R44	1092.007	42.57	39.24	7.8

R46	1092.958	29.49	29.20	1.0
R48	1093.885	20.02	21.36	-6.7
R50	1094.786	15.21	15.37	-1.1
R56	1097.345	5.22	5.36	-2.7
R58	1098.149	3.64	3.49	4.0

Units are 10^{-25} cm/mol at 296 K in natural abundance. σ are the line positions in cm^{-1} . S_{obs} are the measured intensities and S_{calc} the intensities calculated using the transition moment constants listed in Table VI. % is the relative difference between these two values.

TABLE IV

Line	σ	S_{obs}	S_{cal}	%
P27	904.102	4.94	5.02	-1.6
P26	904.765	5.34	5.35	-0.1
P25	905.950	5.89	5.64	4.2
P24	906.639	5.93	5.98	-0.9
P22	908.487	6.77	6.55	3.3
P21	909.578	6.71	6.82	-1.6
P20	910.310	6.78	7.00	-3.3
P19	911.360	7.05	7.17	-1.8
P18	912.108	7.37	7.31	0.8
P17	913.118	7.21	7.40	-2.6
P16	913.880	7.23	7.41	-2.5
P15	914.854	7.30	7.40	-1.3
P12	917.350	7.29	6.88	5.6
P11	918.258	6.47	6.62	-2.3
P 9	919.927	5.92	5.88	0.8
P 7	921.573	4.83	4.82	0.3
P 6	922.366	4.26	4.19	1.8
R 3	930.223	2.87	2.86	0.5
R 8	933.917	6.15	6.02	2.1
R10	933.350	6.93	6.87	0.9
R11	936.086	6.97	7.20	-3.3
R16	939.496	8.01	7.80	2.6
R19	941.584	7.80	7.49	4.0
R22	943.412	6.95	6.77	2.6
R27	946.715	5.13	5.13	0.0
R28	947.096	4.68	4.78	-2.0

Units are 10^{-25} cm/mol at 296 K in natural abundance. σ are the line positions in cm^{-1} . S_{obs} are the measured intensities and S_{calc} the intensities calculated using the transition moment constants listed in Table VI. % is the relative difference between these two values.

TABLE V

Line	σ	S_{obs}	S_{cal}	%
P41	1034.412	2.17	2.16	0.4
P39	1036.460	2.77	2.80	-1.1
P38	1036.927	3.19	3.16	0.8
P37	1038.484	3.44	3.56	-3.4
P33	1042.462	5.50	5.47	0.6
P31	1044.415	6.81	6.58	3.3
P29	1046.344	7.75	7.77	-0.3
P27	1048.248	8.91	8.99	-0.9
P22	1052.702	11.90	11.85	0.4
P20	1054.552	12.70	12.69	0.0
P16	1058.172	13.30	13.44	-1.0
P14	1059.940	13.30	13.17	1.0
P12	1061.681	12.70	12.50	1.6
P11	1062.600	11.90	12.01	-0.9
P10	1063.394	11.20	11.33	-1.2
P 8	1065.079	9.78	9.75	0.3
P 4	1068.366	5.15	5.14	0.1
R 2	1073.850	2.64	2.61	1.3
R 6	1076.829	9.16	9.07	1.0
R11	1080.427	13.10	13.33	-1.8
R13	1081.820	13.60	14.02	-3.1
R18	1085.095	13.80	14.20	-2.9
R20	1086.375	14.20	13.61	4.2
R23	1088.403	12.30	12.15	1.2
R25	1089.645	11.20	10.88	2.9
R27	1090.861	9.50	9.62	-1.2
R28	1091.215	8.75	8.95	-2.2
R30	1092.356	7.73	7.71	0.3
R32	1093.470	6.48	6.41	1.0
R38	1096.646	3.35	3.39	-1.2

Units are 10^{-25} cm/mol at 296 K in natural abundance. σ are the line positions in cm^{-1} . S_{obs} are the measured intensities and S_{calc} the intensities calculated using the transition moment constants listed in Table VI. % is the relative difference between these two values.

TABLE VI

σ_0	Transition	μ_0^2 10 ⁻³ Debye ²	A_1 x10 ⁴	A_2 x10 ⁵
927.156	01111-11101	1.4344 (37)	-5.6 (20)	
960.959	00011-10001	1.4395 (55)	-7.83 (41)	-1.06 (13)
1063.735	00011-10002	1.1774 (24)		1.33 (17)
1071.542	01111-11102	1.123 (66)	-1.0 (7)	

σ_0 is the band center in cm⁻¹. The uncertainties are two standard deviations in units of the last digit.

TABLE VII

σ_0	Transition	S_v This work	S_v DND	% ^a	S_v HITRAN'86	% ^b
927.156	01111-11101	4.14	4.20	1.4	4.20	1.4
960.959	00011-10001	61.3	61.5	0.3	68.7	12.1
1063.735	00011-10002	91.5	91.3	-0.2	97.5	6.6
1071.542	01111-11102	7.57	7.68	1.5	7.68	1.5

Units are 10^{-23} cm/mol at 296 K in natural abundance. σ_0 is the band center in cm^{-1} .
DND Comes from Ref. (2), and HITRAN'86 from Ref. (3)

^a $100 [S_v(\text{DND}) - S_v(\text{this work})] / S_v(\text{this work})$

^b $100 [S_v(\text{HITRAN'86}) - S_v(\text{this work})] / S_v(\text{this work})$

TABLE VIII

Line	00011-10001	00011-10002
P54	71.4	
P52	69.6	
P50	72.8	
P44	73.3	74.8
P42		73.9
P40	78.6	77.7
P38	78.5	80.4
P36	85.0	83.6
P34	84.8	82.7
P32	85.5	88.1
P30	88.5	88.1
P28	85.4	90.9
P26		94.2
P24	93.6	98.6
P22	95.7	99.7
P20		99.2
P18	99.5	99.8
P16	102.3	101.1
P14	103.0	103.5
P12	107.9	103.7
P10	106.8	108.4
P 8	107.2	112.6
P 6	111.4	113.3
P 4	118.4	116.1
P 2	119.7	
R 0	129.6	
R 2	118.2	118.4
R 4	114.0	112.9
R 6	110.2	110.3
R 8	107.5	110.3
R10	106.3	106.9
R12	102.6	103.3
R14	102.0	
R16	100.6	103.3
R18	98.1	96.4
R20	97.4	97.7
R22	95.4	94.4
R24	93.8	
R26	90.2	89.9
R28	88.3	89.0
R30	88.5	88.9
R32	85.7	86.1
R34	82.0	
R36	79.9	82.2
R38	79.8	80.3

R40	78.4	
R42	77.9	77.5
R44	73.2	
R46	72.9	75.8
R48	70.4	68.9
R50	70.0	
R52	70.5	
R54	68.5	
R56	66.9	

CAPTIONS OF THE FIGURES

FIG. 1. Portion of a channeled spectrum (number 4 of Table I), showing fringes caused by multiple optical reflections on the beamsplitter.

FIG. 2. The same spectral region as in Fig. 1, but with saturated lines (spectrum number 1 of Table I). Note that the zero transmission level is also affected by the channel: its true position can be obtained from the top of saturated lines.

FIG. 3. Variation of $|\mu|^2$ (in 10^{-2} Debye²) vs m in the P- and R-branches of the 00011 $\leftarrow$ 10001 band of $^{12}\text{C}^{16}\text{O}_2$. The curve represents the variation of $|\mu|^2$ calculated using the transition moment constants listed in Table VI.

FIG. 4. Variation of $|\mu|^2$ (in 10^{-2} Debye²) vs m in the P- and R-branches of the 00011 $\leftarrow$ 10002 band of $^{12}\text{C}^{16}\text{O}_2$. The curve represents the variation of $|\mu|^2$ calculated using the transition moment constants listed in Table VI.

FIG. 5. Variation of $|\mu|^2$ (in 10^{-2} Debye²) vs m in the P- and R-branches of the 00111 $\leftarrow$ 11101 band of $^{12}\text{C}^{16}\text{O}_2$. The curve represents the variation of $|\mu|^2$ calculated using the transition moment constants listed in Table VI.

FIG. 6. Variation of $|\mu|^2$ (in 10^{-2} Debye²) vs m in the P- and R-branches of the 00111 $\leftarrow$ 11102 band of $^{12}\text{C}^{16}\text{O}_2$. The curve represents the variation of $|\mu|^2$ calculated using the transition moment constants listed in Table VI.

FIG. 7. Variation of the self-broadening coefficients γ of $^{12}\text{C}^{16}\text{O}_2$, in $10^{-3} \text{ cm}^{-1} \cdot \text{atm}^{-1}$, vs $|m|$. The measured values have been plotted as stars for the 00011 $\leftarrow$ 10001 band, and as open triangles for the 00011 $\leftarrow$ 10002 band.

FIGURE 1

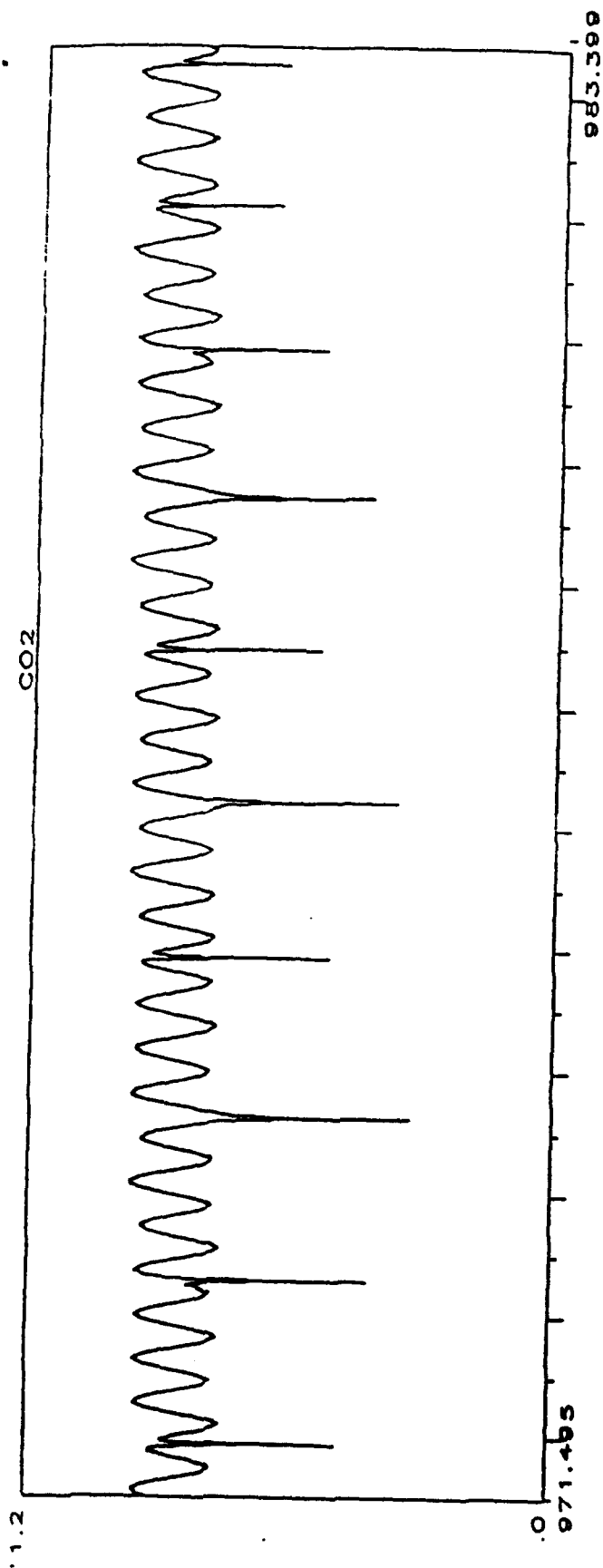


FIGURE 2

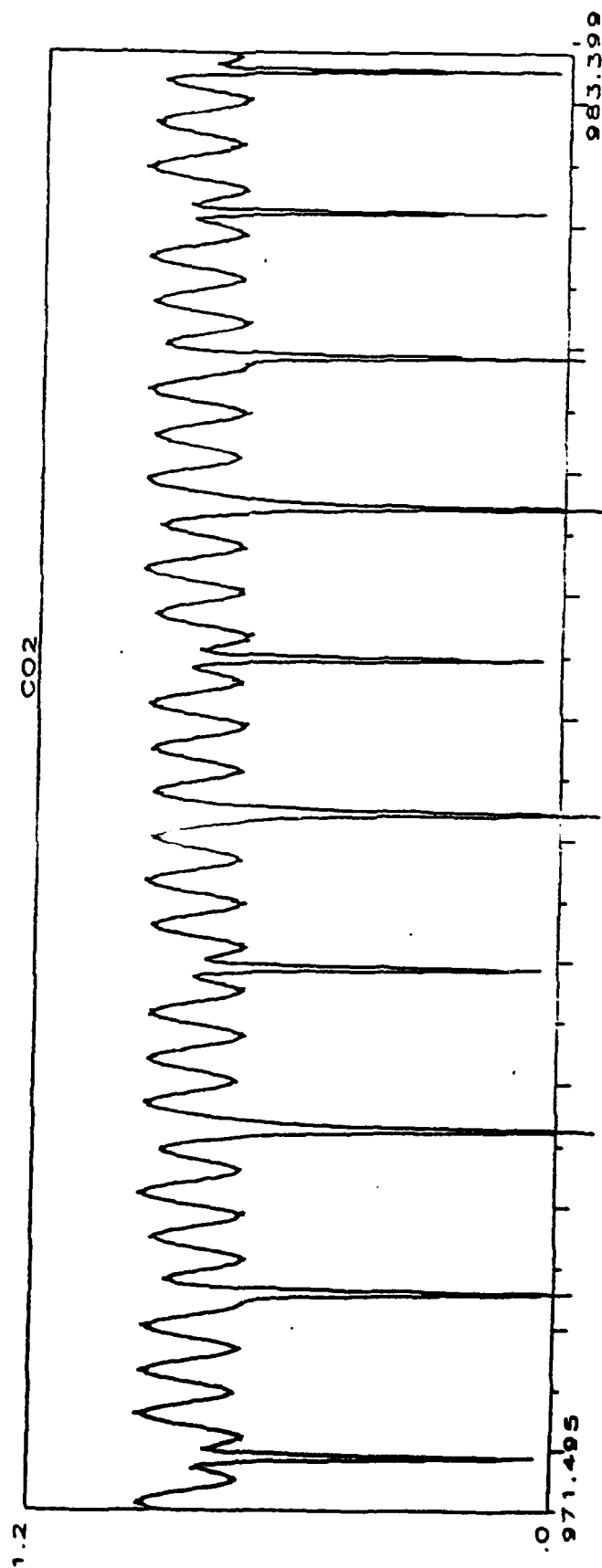


FIGURE 3

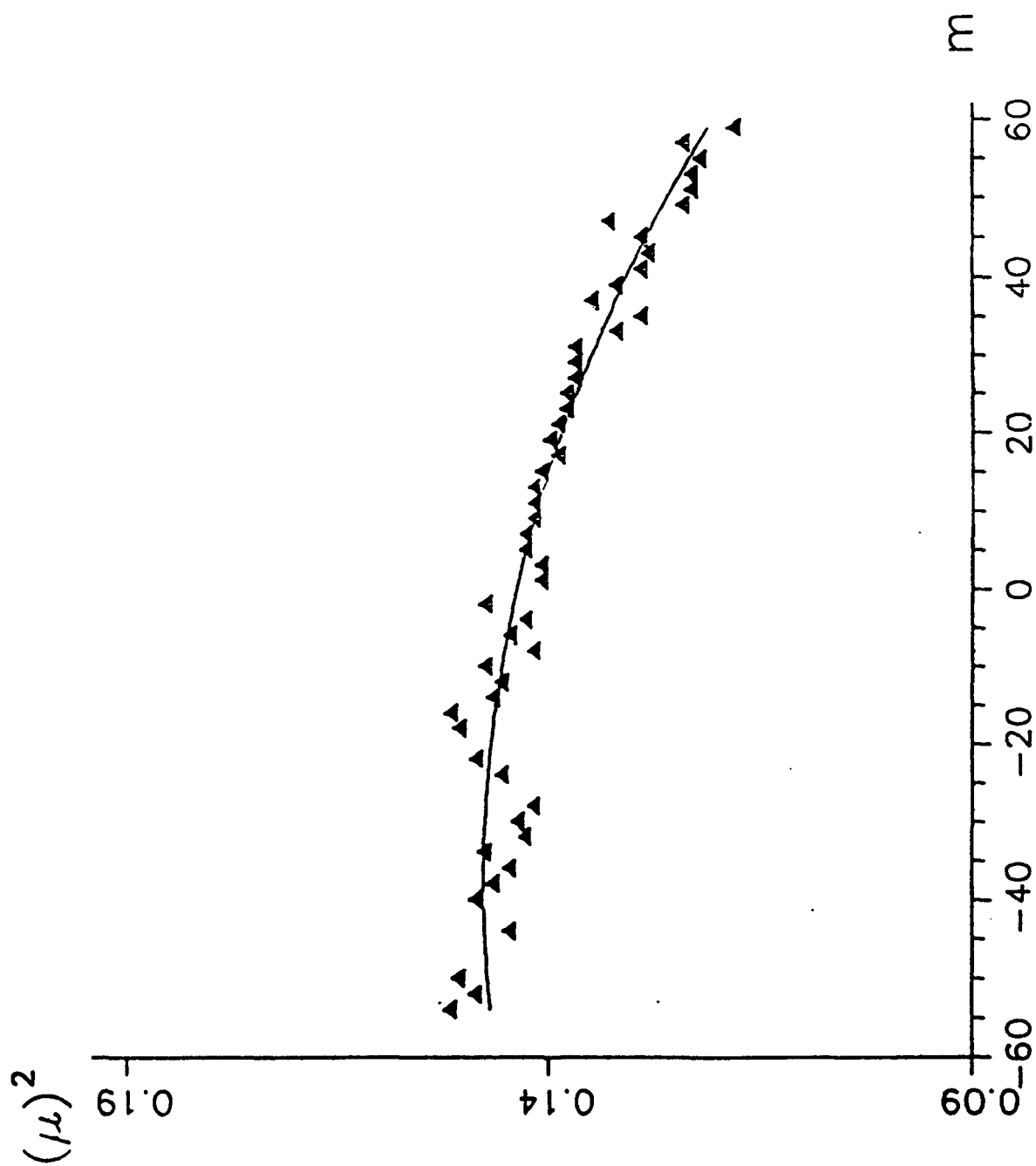


FIGURE 4

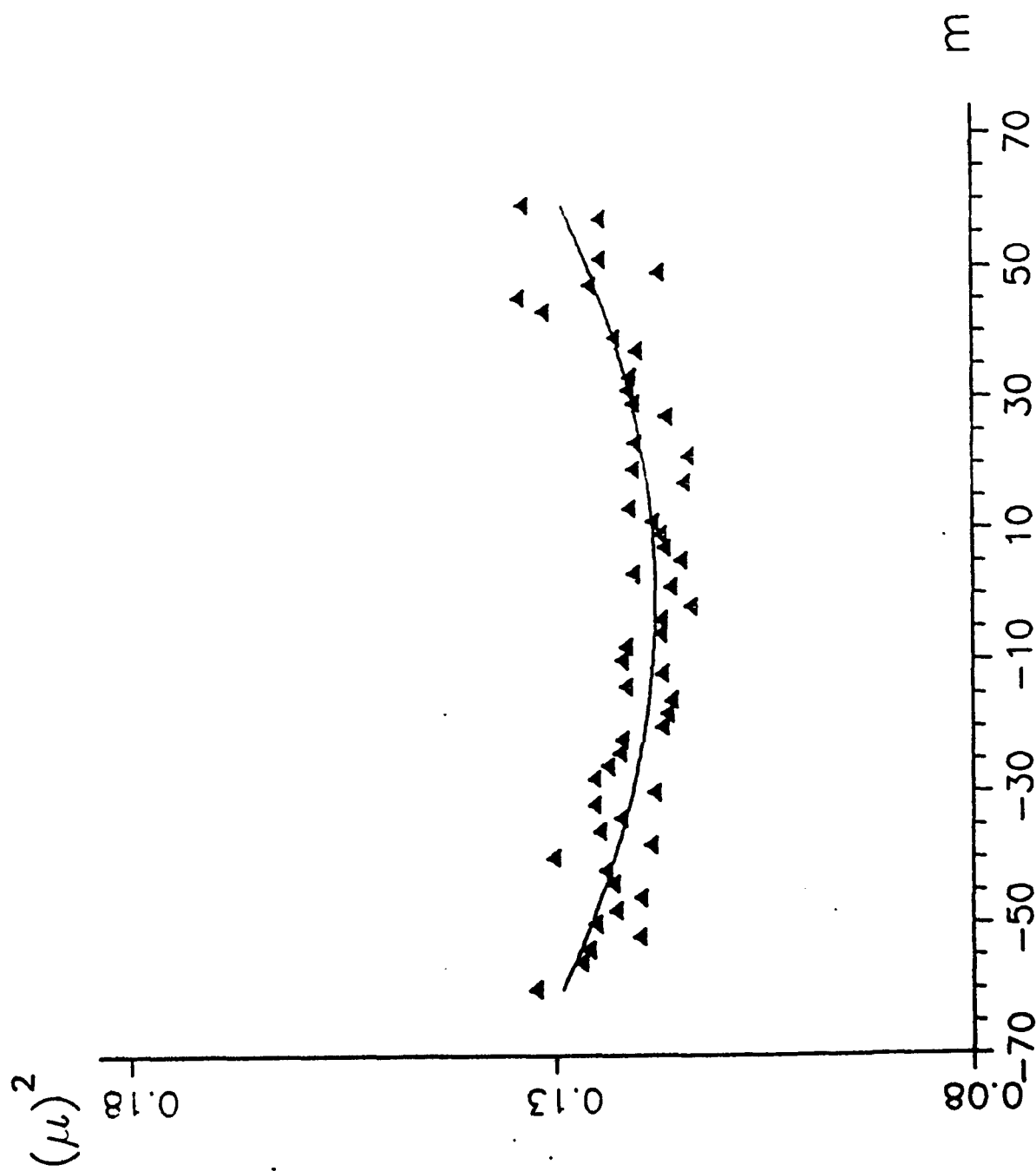


FIGURE 5

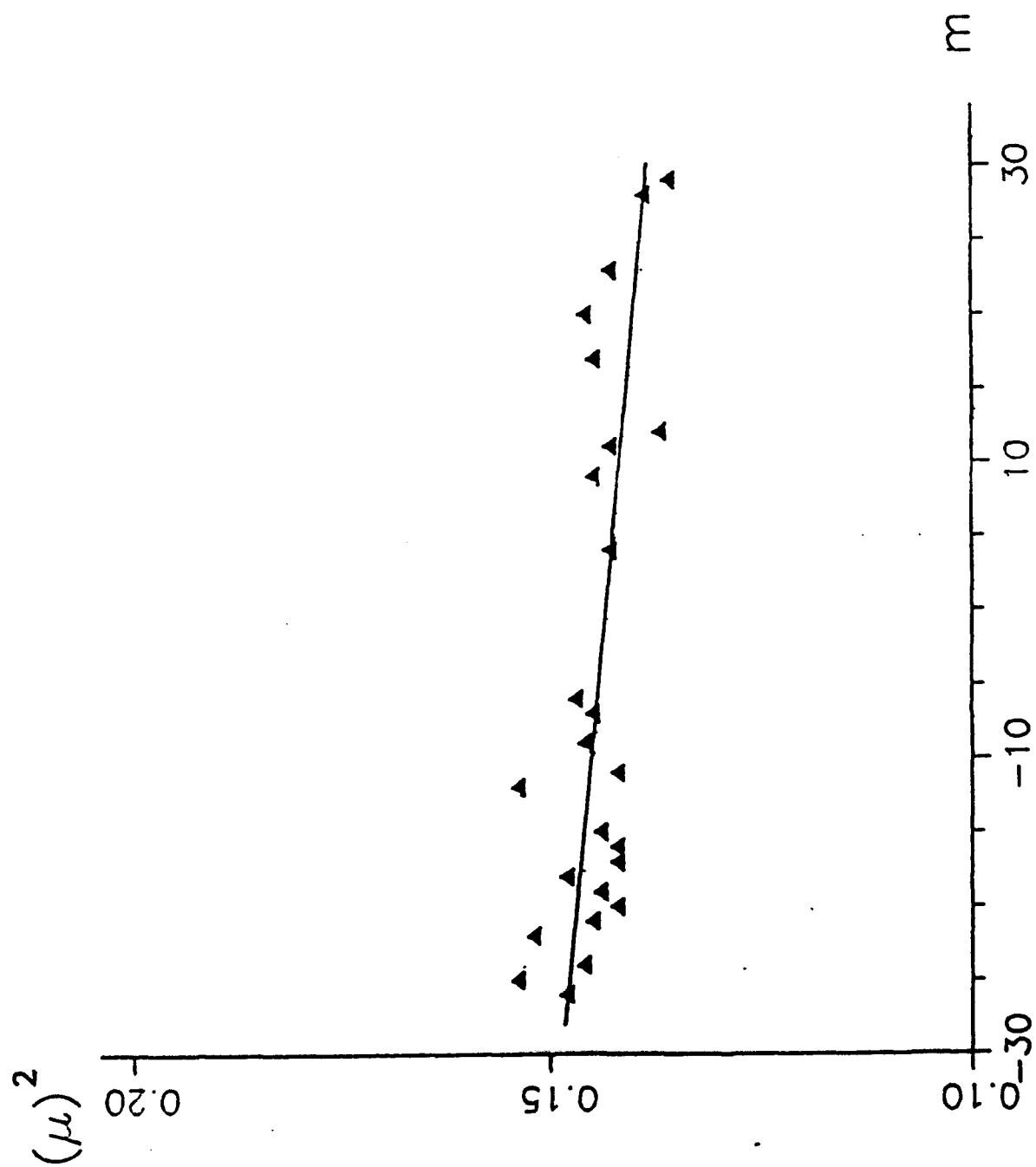


FIGURE 6

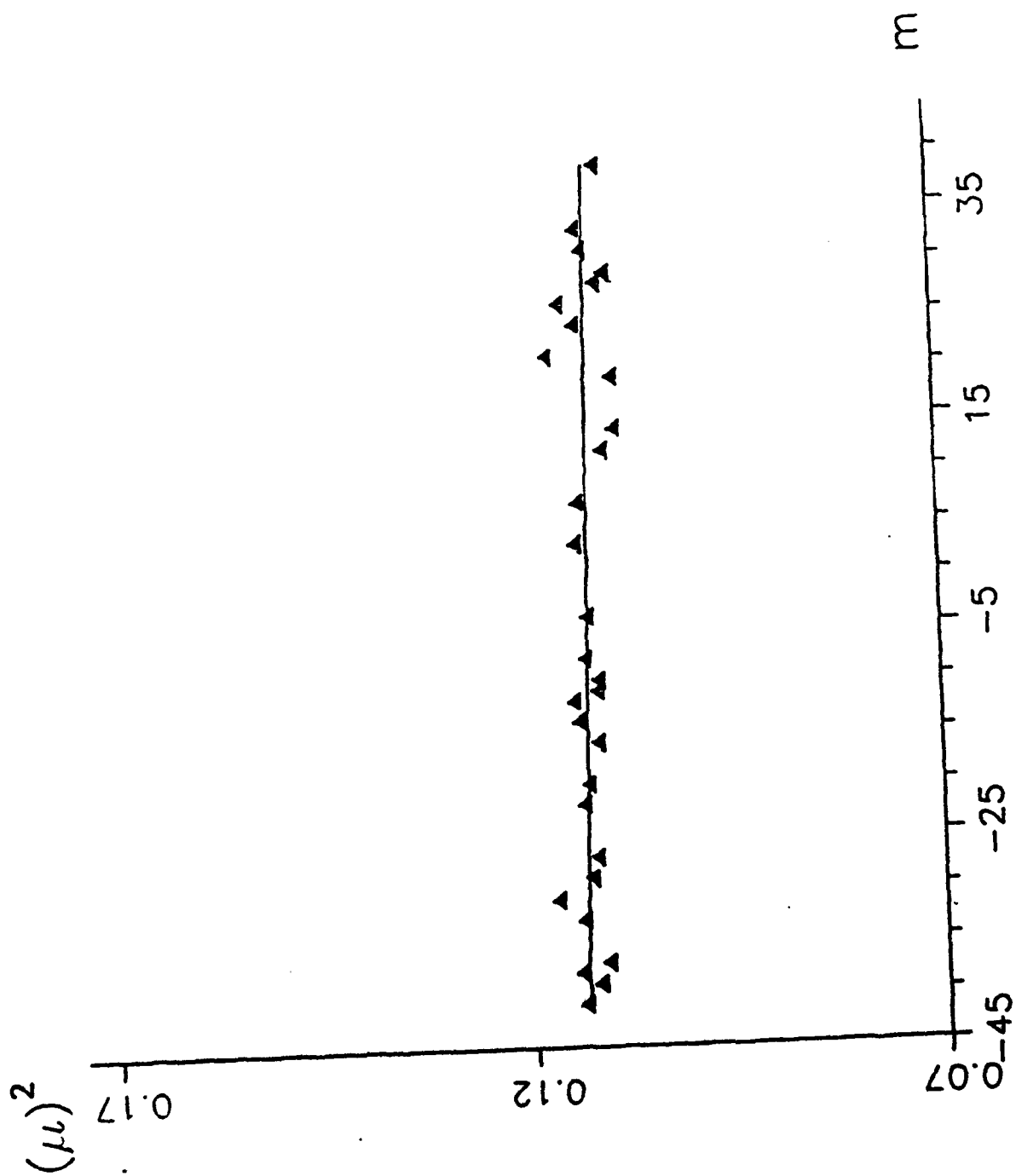
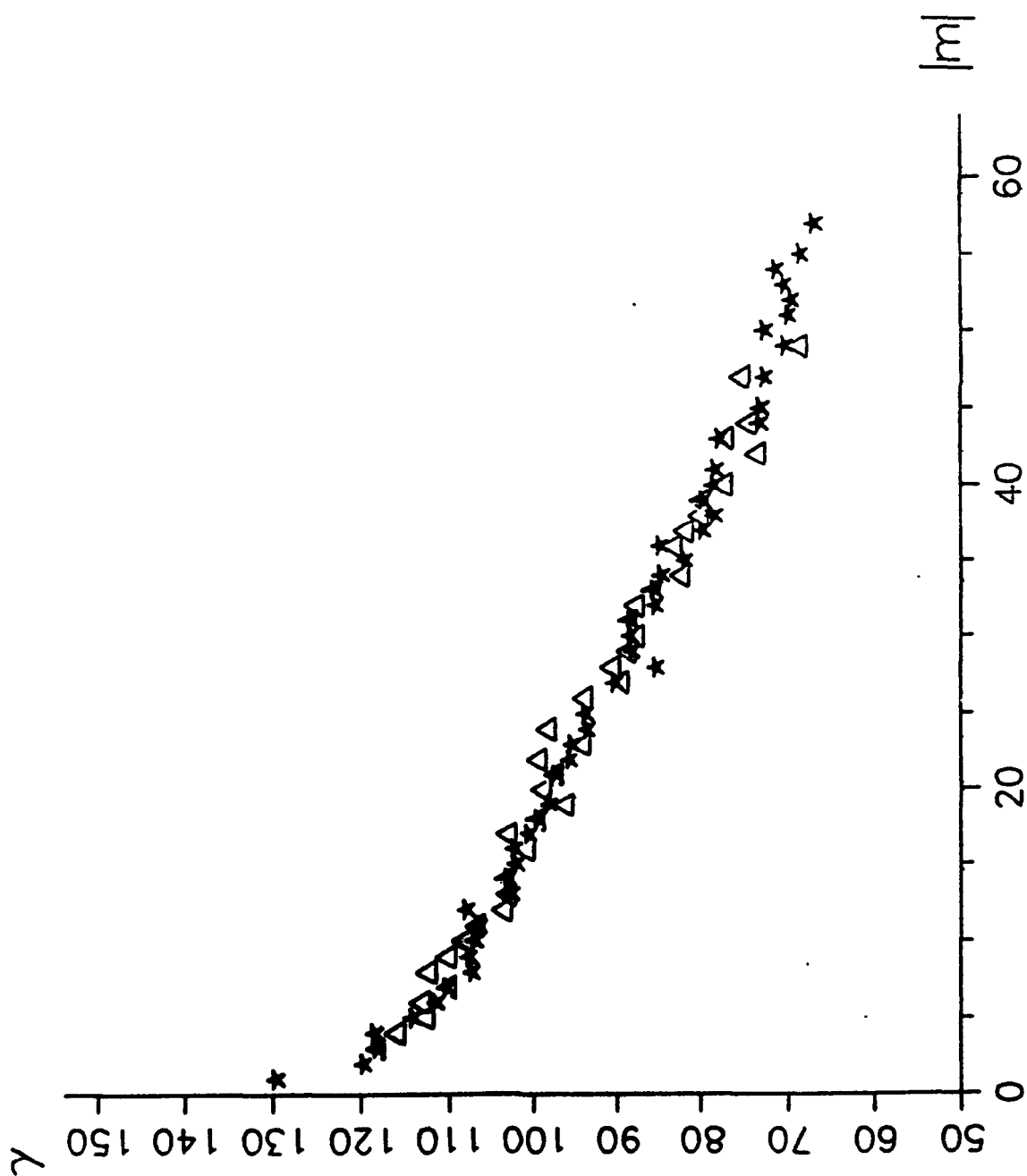


FIGURE 7



PART II

Intensities and Self-Broadening Coefficients of $^{13}\text{C}^{16}\text{O}_2$ Lines in the Laser Band Region

SUMMARY

The intensities of $^{13}\text{C}^{16}\text{O}_2$ lines have been measured in the three bands centered at 883.145, 913.425, and 1017.659 cm^{-1} , using Fourier transform spectra. The square of the transition dipole moment and Herman-Wallis coefficients have been determined. In addition, the self-broadening coefficients of 75 lines have been measured in the two strongest bands.

I. INTRODUCTION

In a previous paper (1), we have studied the laser band region of the main isotopic species $^{12}\text{C}^{16}\text{O}_2$ of carbon dioxide. The study of $^{13}\text{C}^{16}\text{O}_2$, i.e. the most abundant isotopic species after $^{12}\text{C}^{16}\text{O}_2$, is also of interest for atmospheric studies and theoretical purposes. In the laser band region, $^{13}\text{C}^{16}\text{O}_2$ gives rise to two strong parallel hot bands: the 00011-10001 and 00011-10002 bands centered respectively at 913.425 and 1017.659 cm^{-1} . Another weak hot band can also be studied: it is the 01111-11101 band centered at 883.145 cm^{-1} . The last published experimental results concerning these bands are those of Abubakar and Shaw (see Ref. (2) and its bibliography where the references of earlier works can be found). The last published intensity calculations concerned $^{12}\text{C}^{16}\text{O}_2$: they were performed by Wattson and Rothman (3) who used a Direct Numerical Diagonalization method (hereafter denoted as DND). At the present time, the data available through the 1991 version of the HITRAN database (4) are currently used for various radiative transfer studies.

We present here the results of systematic measurements of line intensities in the three above-mentioned bands. High resolution Fourier transform spectra (unapodized FWHM = $2.7 \times 10^{-3} \text{ cm}^{-1}$) have been used to retrieve accurate absolute line and band intensities. The self-broadening coefficients of 75 lines pertaining to the two strongest bands could also be measured: as for the main isotopic species, they do not reveal any vibrational nor isotopic dependences.

II. EXPERIMENTAL DETAILS

The intensity and self-broadening coefficient measurements were performed on five spectra recorded with the Fourier transform spectrometer of the Laboratoire de Physique Moléculaire et Applications, at the Université Paris-Sud. The experimental conditions are summarized in Table I.

The length of the absorption path inside the White-type cell is very well known, so that the uncertainty on this quantity ($\approx 0.1\%$) has very small effects on the retrieved line parameters. Since hot bands have been studied in this work, it was necessary to know with a high precision the temperature of the absorbing gas. For that, the temperature was measured in three places: in the room, on the cell walls, and inside the cell. The equality of the three measured values has shown that a thermal equilibrium had been reached during the recording of each interferogram. However, as a recording takes around ten hours, small variations of the temperature occur. Then, some significant improvements were brought to the experimental setup, in order to know accurately the variation of the temperature inside the cell during the recording of the interferogram, and it was checked that these variations were very small, as it can be seen in Table I, where the uncertainties in the temperature take into account both the uncertainty due to the measurement (about 0.1 K) and the variation of the temperature. In the same way, the uncertainty of 2×10^{-4} atm on the total pressure takes also into account the very small variations of this pressure, due to the variations of the temperature.

The ^{13}C -enriched carbon dioxide sample used was furnished by the Sigma Chemical Company: this sample contained 99 atom % ^{13}C and had a minimum purity of 98%. The recorded spectra showed that this sample is actually also enriched in ^{18}O , since the 10001-00001 band of $^{16}\text{O}^{13}\text{C}^{18}\text{O}$ centered at 1244.900 cm^{-1} occurs. The concentrations of the different isotopic species have been accurately measured by mass spectroscopy, performed at the Laboratoire de Chimie Organique Structurale of the Université Pierre et Marie Curie. A R30-10 Nermag mass spectrometer was used with electron impact ionization mode (70 eV electron energy, 200 mA filament current, and 10 V repeller); the pressure of the source of ^{13}C -enriched sample was 2×10^{-7} torr, and the resolution was 1500. Ten experiment series, each one corresponding to an average of 50 mass spectra, were recorded in similar source conditions. Finally, we found a concentration of $^{13}\text{C}^{16}\text{O}_2$ equal to 0.865 ± 0.020 . This value has been confirmed by intensity measurements, performed on lines pertaining to the $^{12}\text{C}^{16}\text{O}_2$, $^{16}\text{O}^{12}\text{C}^{18}\text{O}$, and $^{16}\text{O}^{13}\text{C}^{18}\text{O}$ isotopic species.

III. METHOD OF MEASUREMENTS

III.1. Treatment of the channeled spectra

In the studied spectral region, fringes, caused by multiple optical reflections on the opposite sides of the beam splitter, appear on the spectra. The presence of a channel of this type is a source of difficulties in the treatment of the spectra, since it has been proved that it could hardly affect the line positions and intensities (5-7). The channel spectra were treated as in our previous work (1).

III.2. The fitting procedure

To obtain the line parameters, a computed spectrum is adjusted to the experimental one. For that, the line shape is assumed to be a Voigt profile, calculated with the aid of the Gautschi's algorithm (8), and the apparatus function takes into account the slight apodization due to the through-put (9), as well as the asymmetry (7) depending upon the position of the studied line with respect to the channel.

The intensity of some lines cannot be measured, since in some spectral regions it was impossible to fit the channel in their vicinity, because of the presence of neighboring lines. (Note that the spectra are somewhat dense in lines, since the lines pertaining to at least four isotopic species are present.)

IV. DATA REDUCTION AND DISCUSSION OF THE RESULTS

IV.1. Line intensities

Using the method detailed in the previous section, we have measured one hundred of line intensities in the laser band region of $^{13}\text{C}^{16}\text{O}_2$. The five spectra (Table I) have been used, and we checked that the lines which could be measured simultaneously in different spectra does not exhibit systematic discrepancies.

Our results are reported in Tables II-IV according to the bands; the intensities have been converted to cm/mol-unit at the reference temperature of the HITRAN database, i.e., 296 K. The uncertainty on these intensities will be discussed now. The treatment of the channel avoid large errors on the line parameters determination, but it decreases slightly the signal to noise ratio. The residuals of the fits are mainly due to the noise. On the average, the statistical relative uncertainties on the obtained intensities is 2 %. An additional uncertainty comes from the uncertainty on the temperature: several tests showed us that an error of 0.25 K on the temperature does not change the intensities by more than 1 %. The greatest source of errors is the uncertainty on the $^{13}\text{C}^{16}\text{O}_2$ concentration, i.e., about 3%. On the whole, a maximum value of the uncertainty on our absolute line intensities is about 7 %.

For each band, we have derived the square of the transition dipole moment $|\mu|^2$, with respect to the running index m ($m = -J''$ in the P branch and $J''+1$ in the R branch, J'' being the rotational quantum number of the lower level). $|\mu|^2$ can be expressed as $|\mu|^2$

$= |\mu_0|^2 F(m)$, where $|\mu_0|^2$ is the vibrational dipole moment matrix element and $F(m)$ the F-factor including Herman-Wallis coefficients:

$$F(m) = [1 + A_1 m + A_2 J''(J''+1)]^2. \quad (1)$$

In addition, the relationship between the intensity of a transition between states i and f , S_{if} , in natural abundance, and $|\mu|^2$ is given by:

$$S_{if}(T) = (8\pi^3/3hc) \sigma_{if} [1 - \exp(-c_2 \sigma_{if} / T)] (I_a/Q(T)) g_n \exp(-c_2 E_i / T) L_{if} |\mu|^2 10^{-36}, \quad (2)$$

where σ_{if} is the frequency of the transition, c_2 is the second radiation constant (hc/k), I_a is the natural isotopic abundance, $Q(T)$ is the total internal partition sum (deduced from Ref. (10)), g_n is the nuclear statistical weight of the lower level (equal to 2 for $^{13}\text{C}^{16}\text{O}_2$), E_i is the energy of the lower state, and L_{if} is the rotational line intensity or Hönl-London factor. The units are cgs, except for $|\mu|$ which is in Debyes. The point to be noted is that in this definition the line intensities are functions of the temperature, T , and the isotopic abundance I_a , while $|\mu|^2$ is independent of these quantities. The transition moment constants obtained through a fit of the line intensities are reported in Table VI. Using Eq. (2), the line intensities have been calculated and compared with their experimental values (see Tables II-IV). The agreement is good, as can also be seen on Figs. 1-3.

From the usual relationship between the band intensity and the

square of the transition dipole moment (3,11), we have calculated the intensities of the four studied bands. The obtained values are reported in Table V.

IV.2. Self-broadening coefficients

The fitting of the line profiles can give simultaneously the line intensities and the self-broadening coefficients. This was done for the two strongest bands, but this could not be possible for the other band because of the weakness of the lines. For these weak hot lines, the self-broadening coefficients were constrained to approximate values, close to those measured in other bands.

The measured self-broadening coefficients are listed in Table VII and plotted on Fig. 4. The temperature is 293.5 ± 0.25 K, and the uncertainty on absolute values is about 5%. Figure 4 shows that for the two concerned bands, no vibrational dependence appears. One can also notice that no isotopic dependence appears, since the results concerning the two molecules $^{12}\text{C}^{16}\text{O}_2$ (1) and $^{13}\text{C}^{16}\text{O}_2$ are very close.

V. CONCLUSION

Using Fourier transform spectra, systematic measurements of absolute line intensities have been performed in the $^{13}\text{C}^{16}\text{O}_2$ laser bands centered at 883.145, 913.425, and 1017.659 cm^{-1} , improving upon the previous experimental results. Also, self-broadening coefficients of lines belonging to the two strongest bands were measured. Together with our previous results (1), these new results, concerning the laser band region of the two main isotopic species of the CO_2 molecule, will be useful for radiative transfer studies and for theoretical purposes.

CAPTIONS OF THE TABLES

TABLE I. Experimental Conditions for the $^{13}\text{C}^{16}\text{O}_2$ spectra

TABLE II. Line Intensities for the 00011-10001 Band of $^{13}\text{C}^{16}\text{O}_2$

Footnote of Table II: Units are 10^{-24} cm/mol at 296 K for pure $^{13}\text{C}^{16}\text{O}_2$. σ are the line positions in cm^{-1} . S_{obs} are the measured intensities and S_{calc} the intensities calculated using the transition moment constants listed in Table V. $\%$ is $100 \times (S_{\text{obs}} - S_{\text{calc}}) / S_{\text{obs}}$.

TABLE III. Line Intensities for the 00011-10002 Band of $^{13}\text{C}^{16}\text{O}_2$

Footnote of Table III: Units are 10^{-24} cm/mol at 296 K for pure $^{13}\text{C}^{16}\text{O}_2$. σ are the line positions in cm^{-1} . S_{obs} are the measured intensities and S_{calc} the intensities calculated using the transition moment constants listed in Table V. $\%$ is $100 \times (S_{\text{obs}} - S_{\text{calc}}) / S_{\text{obs}}$.

TABLE IV. Line Intensities for the 01111-11101 Band of $^{13}\text{C}^{16}\text{O}_2$

Footnote of Table IV: Units are 10^{-24} cm/mol at 296 K for pure $^{13}\text{C}^{16}\text{O}_2$. σ are the line positions in cm^{-1} . S_{obs} are the measured intensities and S_{calc} the intensities calculated using the transition moment constants listed in Table V. $\%$ is $100 \times (S_{\text{obs}} - S_{\text{calc}}) / S_{\text{obs}}$.

TABLE V. Transition Moment Constants $|\mu_0|^2$, A_1 , and A_2 for $^{13}\text{C}^{16}\text{O}_2$

Footnote of Table V: σ_0 is the band center in cm^{-1} . The uncertainties are two standard deviations in unit of the last digit.

TABLE VI. Band Intensities S_ν of the Studied Laser Bands of $^{13}\text{C}^{16}\text{O}_2$

Footnote of Table VI: Units are 10^{-22} cm/mol at 296 K for pure $^{13}\text{C}^{16}\text{O}_2$. σ_0 is the band center in cm^{-1} . HITRAN'91 comes from Ref.

(4)

TABLE VII. Self-Broadening Coefficients Measured for Lines of the 00011-10001 and 00011-10002 Bands of $^{13}\text{C}^{16}\text{O}_2$, in $10^{-3} \text{ cm}^{-1}.\text{atm}^{-1}$

TABLE I

Radius of the iris: 2.85 mm

Focal length of the collimator: 2000 mm

Signal to Noise Ratio: ≈ 150

Absorbing gas: ^{13}C -enriched carbon dioxide, purchased from the Sigma Chemical Company, and containing 99 atom % ^{13}C with 98 % minimum purity. The concentration in $^{13}\text{C}^{16}\text{O}_2$ is 0.865 ± 0.02

Spectrum number	Absorbing path (cm)	Total pressure (10^{-2} atm) $\pm 2 \times 10^{-4}$ atm	Maximal path difference (cm)	Temperature (K)
1	417	5.412	184.19	293.50 ± 0.15
2	1217	5.438	173.06	293.45 ± 0.15
3	2817	5.411	184.19	293.65 ± 0.25
4	5217	5.417	184.19	293.75 ± 0.20
5	5217	5.433	184.19	293.30 ± 0.20

TABLE II

Line	σ	S_{obs}	S_{calc}	$\%$
P52	866.386	0.662	0.695	-5.0
P48	870.484	1.489	1.386	6.9
P46	872.502	1.830	1.913	-4.5
P44	874.499	2.763	2.589	6.3
P42	876.477	3.255	3.445	-5.8
P40	878.434	4.551	4.506	1.0
P38	880.371	5.805	5.793	0.2
P36	882.287	7.111	7.300	-2.7
P34	884.184	8.944	9.040	-1.1
P32	886.061	11.12	10.99	1.2
P30	887.919	13.34	13.10	1.8
P28	889.756	15.36	15.31	0.3
P26	891.574	18.19	17.55	3.5
P22	895.151	22.41	21.57	3.7
P20	896.909	23.04	23.11	-0.3
P18	898.649	23.02	24.11	-4.7
P16	900.369	23.96	24.46	-2.1
P14	902.069	24.72	23.54	4.8
P12	903.750	21.83	22.86	-4.7
P10	905.411	20.39	20.80	-2.0
P8	907.053	17.66	17.88	-1.3
P6	908.675	17.87	18.24	-2.1
P4	910.278	9.653	9.850	-2.0
R4	917.249	12.21	12.22	-0.1
R6	918.744	16.50	16.37	0.8
R8	920.219	20.05	19.82	1.1
R10	921.675	23.22	22.57	2.8
R12	923.111	24.76	24.34	1.7
R14	924.528	25.75	25.27	1.9
R16	925.924	25.18	25.39	-0.8
R20	928.657	23.04	23.60	-2.4
R22	929.993	22.49	21.88	2.7
R24	931.309	19.26	19.80	-2.8
R26	932.605	17.57	17.56	0.1
R28	933.881	15.23	15.27	-0.2
R30	935.136	13.76	12.99	5.6
R32	936.370	10.27	10.83	-5.4
R34	937.584	9.071	8.877	2.1
R36	938.778	7.105	7.126	-0.3
R38	939.950	5.511	5.632	-2.2

TABLE III

Line	σ	S_{obs}	S_{calc}	δ
P58	960.663	0.171	0.166	2.7
P56	963.002	0.245	0.245	0.0
P54	965.317	0.350	0.359	-2.7
P52	967.607	0.514	0.517	-0.7
P50	969.871	0.747	0.734	1.7
P48	972.110	1.076	1.024	4.8
P46	974.323	1.383	1.394	-0.8
P44	976.510	1.823	1.881	-3.2
P42	978.671	2.607	2.486	4.6
P40	980.805	3.332	3.240	2.8
P38	982.913	4.140	4.140	0.0
P36	984.993	4.902	5.216	-6.4
P32	989.073	7.732	7.775	-0.6
P30	991.072	9.166	9.243	-0.8
P28	993.043	10.73	10.78	-0.4
P26	994.986	11.62	12.29	-5.8
P24	996.901	13.59	13.82	-1.7
P22	998.788	15.01	15.12	-0.7
P20	1000.647	16.27	16.11	1.0
P18	1002.478	16.48	16.84	-2.2
P4	1014.488	6.700	6.859	-1.5
R2	1019.961	5.431	5.309	2.3
R4	1021.459	8.769	8.632	1.6
R6	1022.928	11.66	11.63	0.3
R8	1024.368	13.86	14.13	-1.9
R10	1025.778	15.98	16.05	-0.4
R12	1027.160	17.69	17.44	1.4
R14	1028.512	18.16	18.13	-0.1
R16	1029.835	17.95	18.35	-2.2
R20	1032.395	17.54	17.24	1.7
R22	1033.631	16.32	16.07	1.5
R24	1034.838	15.07	14.67	2.6
R26	1036.017	13.28	13.13	1.1
R30	1038.289	10.02	9.825	1.9
R32	1039.382	8.644	8.281	4.2
R38	1042.492	4.554	4.406	3.2
R46	1046.249	1.411	1.495	-6.0
R48	1047.120	1.048	1.093	-4.3

TABLE IV

Line	σ	S_{obs}	S_{calc}	δ
P32	855.527	0.366	0.378	-3.2
P29	858.604	0.505	0.497	1.6
P28	859.273	0.545	0.537	1.4
P27	860.424	0.560	0.576	-1.8
P26	861.115	0.614	0.615	-0.2
P24	862.935	0.695	0.695	0.0
P22	864.734	0.796	0.763	4.1
P21	865.770	0.799	0.796	0.3
P20	866.513	0.824	0.822	0.3
P19	867.514	0.815	0.841	-3.2
P18	868.270	0.867	0.860	0.8
P17	869.240	0.872	0.870	0.3
P16	870.007	0.883	0.870	1.4
P14	871.722	0.876	0.857	2.2
P13	872.634	0.847	0.841	0.7
P12	873.417	0.825	0.814	1.4
P10	875.090	0.719	0.730	-1.6
P9	875.953	0.672	0.681	-1.3
P7	877.584	0.546	0.560	-2.5
R4	886.975	0.389	0.402	-3.3
R6	888.470	0.556	0.543	2.4
R9	890.684	0.676	0.699	-3.4
R14	894.240	0.838	0.808	3.6

TABLE V

σ_0	Transition	$ \mu_0 ^2$ 10^{-3} Debye ²	A_1 $\times 10^4$	A_2 $\times 10^5$
883.145	01111-11101	1.702(14)	-26.4(35)	-6.9(15)
913.425	00011-10002	1.841(15)	-7.8(11)	-1.09(42)
1017.659	00011-10001	0.695(52)	-1.70(85)	1.43(28)

TABLE VI

σ_0	Transition	S_v
		Obs
883.145	01111-11101	0.00634
913.425	00011-10002	0.0907
1017.659	00011-10001	0.0633

TABLE VII

Line	00011-10001	00011-10002
P58		74.7
P56		70.7
P52	70.8	69.6
P50		73.6
P48	72.0	76.0
P46	76.0	72.9
P44	75.2	77.1
P42	78.2	76.7
P40	78.2	78.4
P38		82.0
P36	84.0	77.4
P34	84.1	
P32	84.8	89.4
P30	84.8	89.4
P28	86.7	90.9
P26	91.8	87.9
P24		93.1
P22	97.0	96.3
P20	93.8	99.9
P18	98.1	98.6
P16	100.3	
P14	100.1	
P12	101.3	
P10	105.5	
P8	104.0	
P6	109.4	
P4	115.3	115.9
R2		127.1
R4	110.7	114.1
R6	110.9	108.5
R8	106.4	106.9
R10	105.5	105.9
R12	101.8	104.9
R14	100.7	100.0
R16	97.9	97.8
R20	94.1	97.1
R22	91.1	94.4
R24	91.8	94.9
R26	89.4	92.9
R28	87.8	
R30	89.6	87.5
R32	83.0	86.9
R34	81.9	
R36	79.3	
R38	77.6	82.5
R46		66.8
R48		71.4

CAPTIONS OF THE FIGURES

FIG. 1. Variation of $|\mu|^2$ (in 10^{-2} Debye²) vs m in the P- and R-branches of the 00011 $\leftarrow$ 10001 band of $^{13}\text{C}^{16}\text{O}_2$. The curve represents the variation of $|\mu|^2$ calculated using the transition moment constants listed in Table V.

FIG. 2. Variation of $|\mu|^2$ (in 10^{-2} Debye²) vs m in the P- and R-branches of the 00011 $\leftarrow$ 10002 band of $^{13}\text{C}^{16}\text{O}_2$. The curve represents the variation of $|\mu|^2$ calculated using the transition moment constants listed in Table V.

FIG. 3. Variation of $|\mu|^2$ (in 10^{-2} Debye²) vs m in the P- and R-branches of the 01111 $\leftarrow$ 11101 band of $^{13}\text{C}^{16}\text{O}_2$. The curve represents the variation of $|\mu|^2$ calculated using the transition moment constants listed in Table V.

FIG. 4. Variation of the self-broadening coefficients γ of $^{13}\text{C}^{16}\text{O}_2$, in $10^{-3} \text{ cm}^{-1} \cdot \text{atm}^{-1}$, vs $|m|$. The measured values have been plotted as stars for the 00011 $\leftarrow$ 10001 band, and as open triangles for the 00011 $\leftarrow$ 10002 band.

FIGURE 1

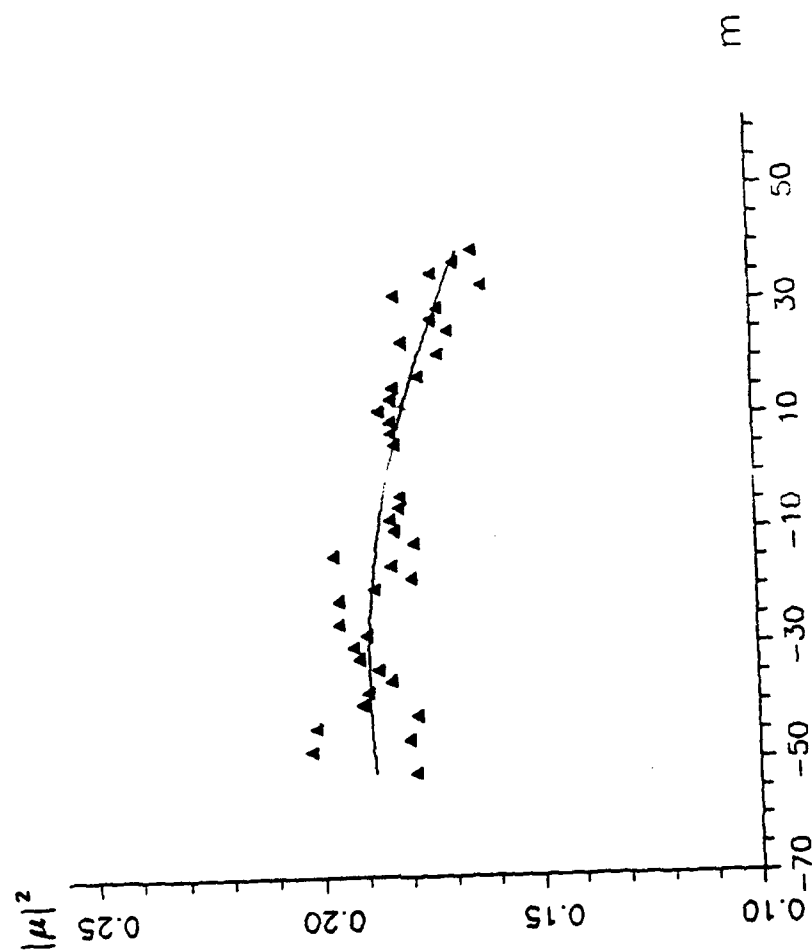


FIGURE 2

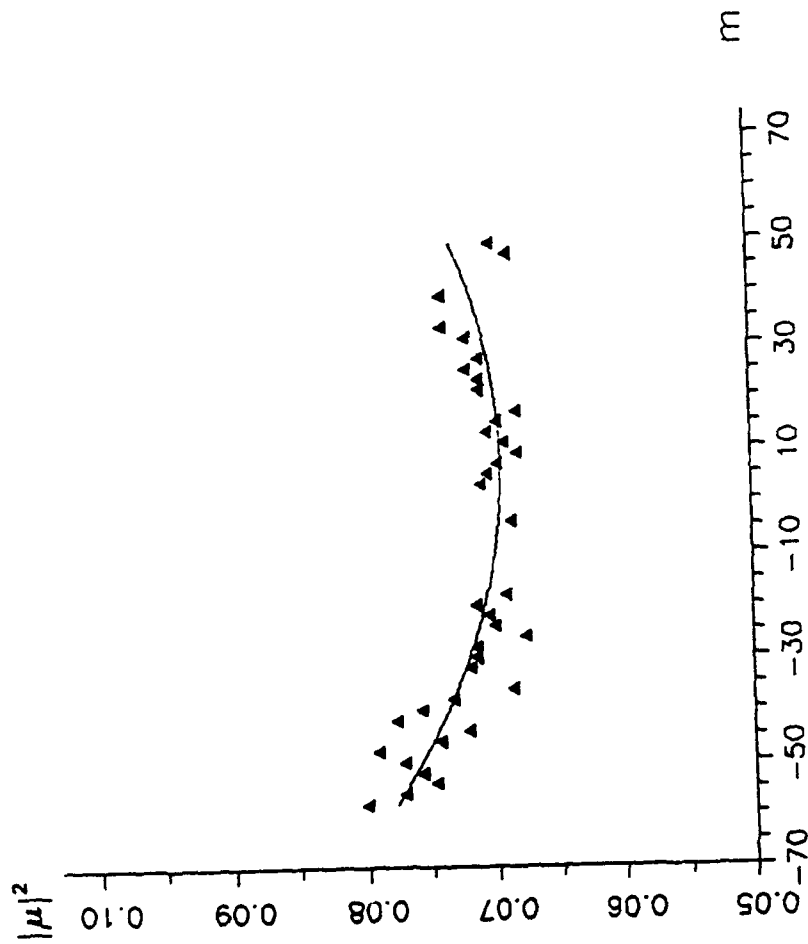


FIGURE 3

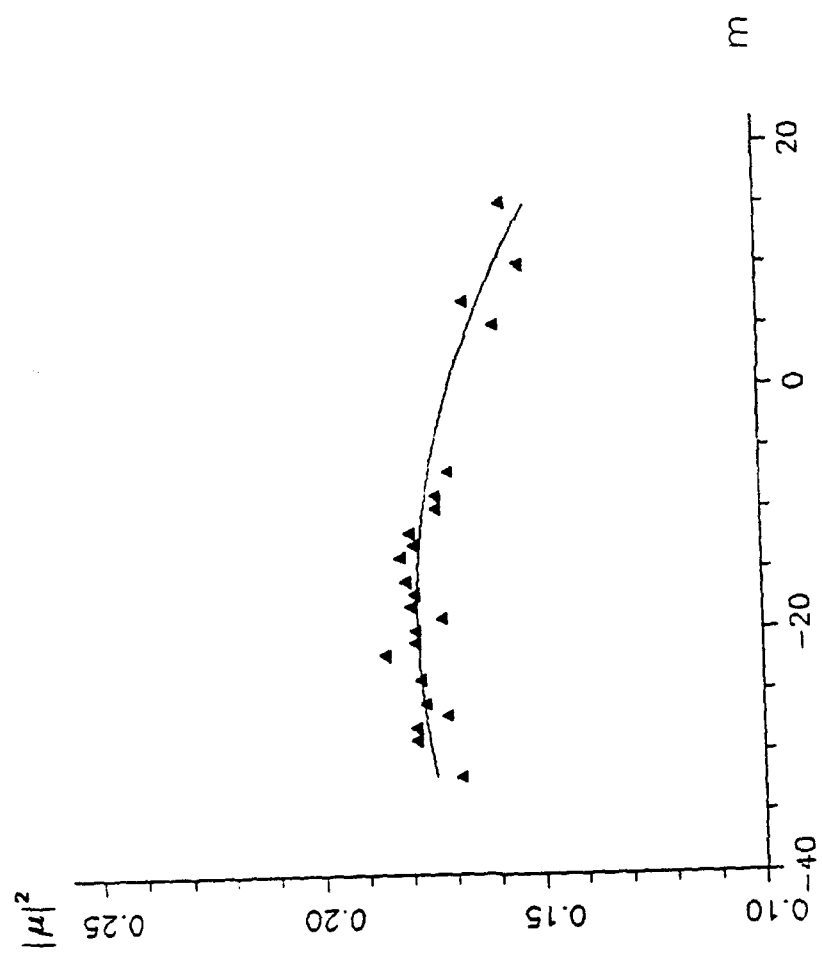
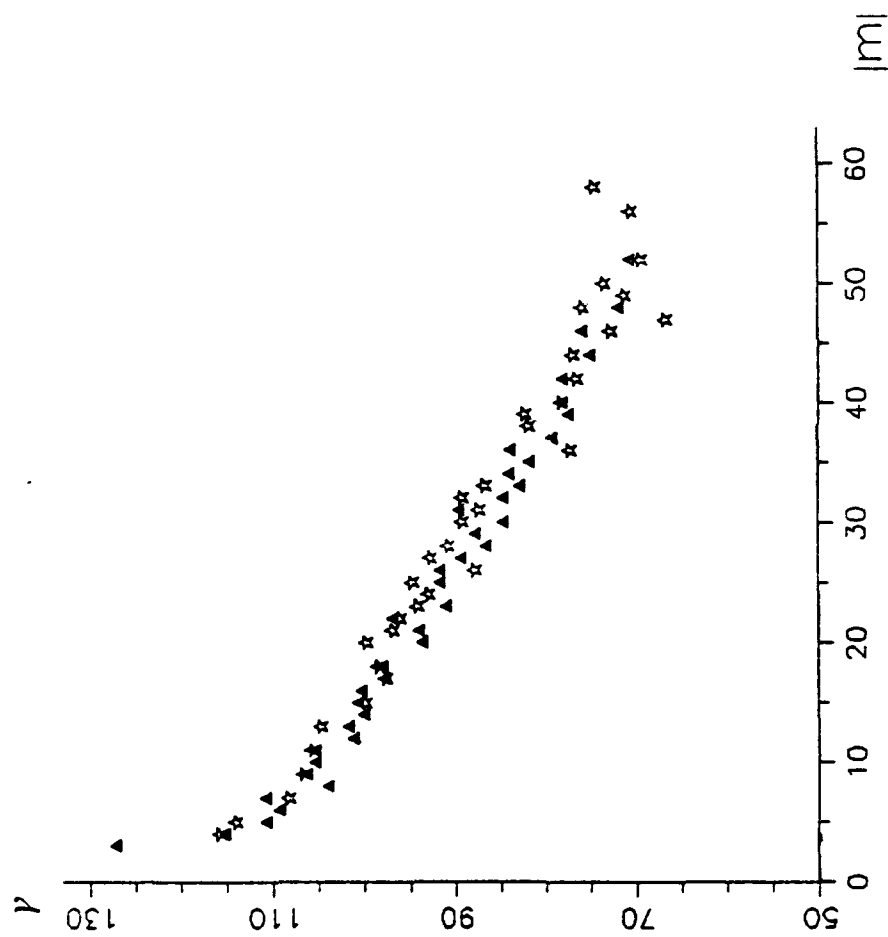


FIGURE 4



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