

Rotational and Vibration Constants of CO[†]

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The spectrum of CO has been observed using a heated absorption tube. J values up to 48 for the 2-0 band and up to ~ 35 for the 3-1 and 4-2 bands were measured. Using previous measurements of the 2-0 band and the results of microwave determinations a set of rotation-vibration constants was deduced. The vibrational constants in vacuum wave numbers are:

$$\omega_e = 2169.8232, \quad \omega_e x_e = -13.2932, \quad \omega_e y_e = 0.01144.$$

The rotational constants are: $B_0 = 1.922\,521$, $D_0 = -6.1193 \times 10^{-6}$, $H_0 = 5.8 \times 10^{-12}$, $\alpha_e = -0.017507$, $\beta_e = 1.0 \times 10^{-9}$, $\gamma_e = 1.0 \times 10^{-6}$. Calculated values for lines in the 5-3, 6-4, and 7-5 bands agree within experimental error with the results of measurement of lines in the solar spectrum.

INTRODUCTION

Several investigations of the infrared spectrum of carbon monoxide have been carried out in the past two decades. Herzberg and Rao (1) in 1949 became the first to photograph the 4-0 band. In 1952, Plyler *et al.* (2) measured absorption lines in the 2-0 and 3-0 bands to an accuracy of $\pm 0.02\text{ cm}^{-1}$. Goldberg and Mueller (3) in 1953 published an extensive investigation in which they identified over 300 lines of CO in the solar spectrum. In 1955 Plyler, Blaine, and Conner (4) measured lines in emission and absorption in the region of 4.67 microns as part of their determination of the velocity of light. Two years later Rank, Guenther, Saksena, Shearer, and Wiggins (5) published interferometric measurements of thirty-three lines of the 2-0 band yielding more precise values of the ground-state constants and making possible a measurement of the velocity of light improved by an order of magnitude. Mould, Price, and Wilkinson (6) in 1960, using infrared emission by a r-f discharge, observed band lines of CO which were well fitted by the most recent values (4, 5) of the vibrational and rotational constants.

In this investigation rotational lines of the 2-0, 3-1, and 4-2 bands of carbon monoxide were measured very precisely and a set of vibrational and rotational constants deduced. The 2-0 band lines measured were from $J = 30$ to $J = 48$. These were then complemented with the lower J -value lines of this band meas-

[†] This research was supported by the National Science Foundation.

ured earlier by Rank *et al.* (5). The rotational lines of the 3-1 band were measured from $J = 0$ to $J = 47$ for the R branch and $J = 1$ to $J = 37$ for the P branch. In the 4-2 band, rotational lines from $J = 2$ to $J = 31$ in the R branch and from $J = 2$ to $J = 23$ in the P branch were measured.

EXPERIMENTAL

Used in this investigation was the 5-meter echelle-type spectrograph described in detail by Rank, Saksena, Skorinko, Eastman, Wiggins, and McCubbin (7) and by Rank, Eastman, Birtley, Skorinko, and Wiggins (8). A 4-in. \times 8-in. Bausch and Lomb transfer grating ruled with 73.25 lines per mm with a blaze angle of approximately 63° was used in a double pass arrangement.

Depending on the particular band line being measured, standard wavelengths in N_2O , HCN, or CO itself were used. More than 600 absorption lines of these gases have been measured by Rank, Skorinko, Eastman, and Wiggins (9), and by Rank, Eastman, Rao, and Wiggins (10). The estimated accuracy of the calculated values of these lines is $\pm 0.001 \text{ cm}^{-1}$.

This investigation was prompted by the construction in this laboratory of a modification of the King's furnace (11) as a source. The radiation from this source is most intense, simulating that of a black body at 3000° .

A 1.3-meter absorption tube with fluorite windows contained the gas at pressures up to 2 cm Hg. It could be heated to a temperature of about 1000°C .

DETERMINATION OF MOLECULAR CONSTANTS

In the course of the analysis of the various bands, some of the molecular constants as determined by least squares treatment yielded values which seemed physically untenable. The reason was suspected to lie in the statistical fluctuation of the data. For this reason values of some of the constants were selected in the manner indicated below rather than by least squares treatment.

THE 2-0 BAND

Rank *et al.* (5) have used the well-known combination relations $\Delta_2 F''(J) \equiv R(J-1) - P(J+1)$ and $\nabla_+(J) \equiv R(J-1) + P(J)$ on their interferometrically measured lines. From a statistical least squares treatment they were able to obtain the ground-state molecular constants from the 2-0 band. They maintain in their paper that the $\Delta_2 F''(J)$ values used in calculating the D_0 and B_0 terms all have a precision well in excess of 1 part in 10^5 .

Employing expressions from the theory of Dunham (12), values for D_0 and H_0 were calculated. Precise values for D_2 and B_2 and ν_0 were also determined by least squares treatment of the data. The values, expressed in wave numbers, which were obtained by them (5) are:

$$B_0 = 1.922521, \quad B_2 = 1.887513,$$

$$D_0 = -6.1193 \times 10^{-6}, \quad D_2 = -6.1174 \times 10^{-6},$$

$$H_0 = H_2 = 5.8 \times 10^{-12}, \quad \nu_0 = 4260.0646.$$

The newly measured lines of the 2-0 band were calculated using the above constants and the equation:

$$\begin{aligned} \nu = \nu_0 &+ (B' + B'')m + (B' - B'' + D' - D'')m^2 \\ &+ [2(D' + D'') + H' + H'']m^3 \\ &+ (D' - D'')m^4 + 3(H' + H'')m^5, \end{aligned} \quad (1)$$

where $m = J + 1$ for the R branch and $= -J$ for the P branch. A comparison of the calculated lines with the observed lines is given in Table I. The probable error is $\pm 0.0023 \text{ cm}^{-1}$. This compares favorably with a probable error of $\pm 0.0020 \text{ cm}^{-1}$ using constants from a least squares fit of the upper and lower states. Although the probable error, of course, is less using the constants from the fitting process, the values of $H_0 = H_2$ and ΔD_{2-0} obtained by this fitting seemed physically unrealistic.

The values for the function $\Delta_2 F''$ for the ground state as determined from

TABLE I
CALCULATED AND OBSERVED FREQUENCIES IN VACUUM WAVE NUMBERS OF THE 2-0
BAND OF CO FROM $J = 29$ TO $J = 49$

J	R(J)		C - O $\times 10^4$	P(J)		C - O $\times 10^4$
	Calc	Obs		Calc	Obs	
29	4342.2000	4342.1961	+39			
30	4343.8066	4343.8088	-22	4114.9179	4114.9157	+22
31	4345.3387	4345.3333	+54	4109.0407	4109.0444	-35
32	4346.7961	4346.7935	+26	4103.0981	4103.0957	+24
33	4348.1787	4348.1802	-15	4097.0912	4097.0903	+9
34	4349.4864	4349.4835	+29	4091.0171	4091.0106	+65
35	4350.7189	4350.7169	+20	4084.8789	4084.8754	+35
36	4351.8762	4351.8780	-18	4078.6759	4078.6755	+4
37	4352.9582	4352.9591	-9	4072.4082	4072.4086	-4
38	4353.9646	4353.9599	+47	4066.0759	4066.0734	+25
39	4354.8953	4354.8892	+61	4059.6791	4059.6819	-28
40	4355.7502	4355.7480	+22	4053.2180	4053.2156	+24
41	4356.5292	4356.5275	+17	4046.6928	4046.6840	+88
42	4357.2321	4357.2264	+57	4040.1036	4040.1033	+3
43	4357.8587	4357.8631	-44	4033.4505	4033.4407	+98
44	4358.4090	4358.4137	-47	4026.7337	4026.7309	+28
45	4358.8828	4358.8843	-15	4019.9534	4019.9434	+100
46	4359.2799	4359.2823	-24	4013.1096	4013.1055	+41
47	4359.6002	4359.6024	-22	4006.2025	4006.1908	+117
48	4359.8436	4359.8493	-57	3999.2323	3999.2294	+29
49				3992.1991	3992.1988	+3

TABLE II
CALCULATED AND OBSERVED VALUES OF $\Delta_2 F''$ IN VACUUM WAVE NUMBERS OBTAINED FROM
THE 2-0 BAND OF CO

J	$\Delta_2 F''$ Calc	$\Delta_2 F''$ Obs	$C - O \times 10^4$
30	233.1592	0.1517	+75
31	240.7086	0.7131	-45
32	248.2485	0.2430	+55
33	255.7791	0.7829	-38
34	263.2998	0.3048	-50
35	270.8104	0.8080	+24
36	278.3107	0.3083	+24
37	285.8004	0.8046	-42
38	293.2791	0.2772	+19
39	300.7466	0.7443	+23
40	308.2025	0.2052	-27
41	315.6467	0.6447	+20
42	323.0787	0.0868	-81
43	330.4982	0.4955	+27
44	337.9053	0.9197	-144
45	345.2994	0.3082	-88
46	352.6802	0.6935	-133
47	360.0475	0.0529	-54
48	367.4011	0.4036	-25
49	374.7405		

measurements are listed in Table II. Also shown here are values calculated from the highly precise constants given by Rank *et al.* (5). The measured results show a probable error of $\pm 0.0032 \text{ cm}^{-1}$ when compared with the calculated values. Although some reduction in the probable error would follow from a least squares treatment, the value of H_0 obtained in this way was much larger than the Dunham value and seemed unreasonable.

Jones and Gordy (13) have reported measurements for CO up to the $5 \rightarrow 6$ rotational transition. Using $c = 299,792.7 \text{ km/sec}$ (14), the values corresponding to B_0 and D_0 are 1.922527 and $6.1342 \times 10^{-6} \text{ cm}^{-1}$. We can compare the observed values for $\Delta_2 F''$ with values calculated from the microwave constants assuming $H'' = 5.8 \times 10^{-12} \text{ cm}^{-1}$. The result of this comparison is that the probable error is nearly twice as large as noted above and the residuals are predominately of one sign. To remedy this a value of $H'' \cong 12 \times 10^{-12}$ would have to be used. It is not clear how this discrepancy between the infrared and microwave results can be resolved. Work now in progress at The Ohio State University (15) may indicate the source of the discrepancy.

THE 3-1 AND 4-2 BANDS

The molecular constants for the states $v = 3$ and 4 were determined using the measured frequencies in the 3-1 and 4-2 bands in conjunction with the precise

TABLE III
OBSERVED AND CALCULATED FREQUENCIES IN VACUUM WAVE NUMBERS OF THE
3-1 BAND OF CO

J	$R(J)$ Calc	$R(J)$ Obs	$C - O \times 10^4$	$P(J)$ Calc	$P(J)$ Obs	$C - O \times 10^4$
0	4210.9064	0.8985	+79			
1	4214.5762	0.5742	+20	4203.3564	0.3658	-94
2	4218.1758	0.1797	-39	4199.4765	0.4798	-33
3	4221.7049	0.7000	+49	4195.5270	0.5296	-26
4	4225.1634	0.1671	-37	4191.5078	0.5116	-38
5	4228.5511	0.5489	+22	4187.4192	0.4197	-5
6	4231.8680			4183.2614	0.2582	+32
7	4235.1138	0.1155	-17	4179.0344	0.0340	+4
8	4238.2885	0.2934	-49	4174.7385	0.7407	-22
9	4241.3918	0.4025	-107	4170.3737	0.3780	-43
10	4244.4236			4165.9402	0.9400	+2
11	4247.3839	0.3532	+307	4161.4383	0.4525	-142
12	4250.2723	0.2626	+97	4156.8679	0.8640	+39
13	4253.0889	0.0909	-20	4151.2292		
14	4255.8334	0.8394	-60	4147.5225	0.5222	+3
15	4258.5057	0.5106	-49	4142.7478	0.7497	-19
16	4261.1056	0.0896	+160	4137.9053	0.9050	+3
17	4263.6331	0.6352	-21	4132.9952	0.9987	-35
18	4266.0879			4128.0176	0.0091	+84
19	4268.4699	0.4743	-44	4122.9725	0.9713	+12
20	4270.7790	0.7832	-42	4117.8603	0.8612	-9
21	4273.0150	0.0236	-86	4112.6810	0.6819	-9
22	4275.1778	0.1853	-75	4107.4348	0.4341	+7
23	4277.2673	0.2743	-70	4102.1218	0.1192	+26
24	4279.2832	0.2789	+43	4096.7422	0.7422	0
25	4281.2255	0.2420	-165	4091.2961	0.2933	+28
26	4283.0940	0.0912	+28	4085.7837	0.7863	-26
27	4284.8886			4080.2050	0.2099	-49
28	4286.6090			4074.5603		
29	4288.2552			4068.8497	0.8554	-57
30	4289.8271	0.8253	+18	4063.0735	0.0718	+17
31	4291.3244			4057.2316	0.2341	-25
32	4292.7471	0.7457	+14	4051.3247	0.3269	-27
33	4294.0950	0.1009	-59	4045.3516		
34	4295.3679	0.3704	-25	4039.3136	0.3182	-46
35	4296.5657	0.5679	-22	4033.2108	0.2022	+86
36	4297.6884			4027.0432	0.0530	-98
37	4298.7356	0.7292	+64	4020.8106	0.8114	-8
38	4299.7073	0.6958	+115	4014.5136		
39	4300.6034					
40	4301.4236	0.4146	+90			
41	4302.1680	0.1635	+45			
42	4302.8362					
43	4303.4282					
44	4303.9438					
45	4304.3830	0.3638	+192			
46	4304.7455	0.7322	+133			
47	4305.0312	0.0206	+106			

values of the constants for the $v = 1$ and 2 states. Values for ν_0 in each case were obtained by fitting low J lines. The results were $\nu_{0_{3-1}} = 4207.1680 \text{ cm}^{-1}$ and $\nu_{0_{4-2}} = 4154.4040 \text{ cm}^{-1}$.

The major difficulty in fitting these bands to yield the most physically realistic results is in finding a value for the constant γ_e . A least squares fit to determine the quantity $B' - B''$ from these bands gives values which, in conjunction with the $B' - B''$ value from the 2-0 band, yield the result that γ_e is slightly negative from the 3-1 band data and $\gamma_e = 1.5 \times 10^{-6}$ from the 4-2 band. These results are smaller than $\gamma_e = 2.96 \times 10^{-6}$ reported by Goldberg and Mueller (3), and an order of magnitude less than given by Rank *et al.* (5) which is cer-

TABLE IV
CALCULATED AND OBSERVED FREQUENCIES IN VACUUM WAVE NUMBERS OF
THE 4-2 BAND OF CO

J	$R(J)$ Calc	$R(J)$ Obs	$C - O \times 10^4$	$P(J)$ Calc	$P(J)$ Obs	$C - O \times 10^4$
0	4158.1106					
1	4161.7504			4150.6306		
2	4165.3102	0.2973	+129	4146.7908		
3	4168.8041	0.8002	+39	4142.8710		
4	4172.2277	0.2411	-134	4138.8871		
5	4175.5805	0.5788	+17	4134.8335		
6	4178.8624	0.8627	-3	4130.7107	0.7110	-3
7	4182.0733	0.0727	+6	4126.5188		
8	4185.2130			4122.2579	0.2541	+38
9	4188.2814	0.2764	+50	4117.9282		
10	4191.2784	0.2755	+29	4113.5298	0.5294	+4
11	4194.2037	0.1993	+44	4109.0629		
12	4197.0572			4104.5276	0.5241	+35
13	4199.8429			4099.9240	0.9277	-37
14	4202.5486	0.5509	-23	4095.2564	0.2552	+12
15	4205.1860	0.1874	-14	4090.5128	0.5146	-18
16	4207.7510	0.7543	-33	4085.7055		
17	4210.2436	0.2385	+51	4080.8305	0.8340	-35
18	4212.6636	0.6647	-11	4075.8880	0.8850	+30
19	4215.0108	0.0117	-9	4070.8781	0.8814	-33
20	4217.2851	0.2894	-43	4065.8010	0.8000	+10
21	4219.4863	0.4848	+15	4060.6569		
22	4221.6143			4055.4458	0.4602	-144
23	4223.6689	0.6726	-37	4050.1680	0.1670	+10
24	4225.6500	0.6493	+7			
25	4227.5576					
26	4229.3912					
27	4231.1510	0.1541	-31			
28	4232.8364	0.8395	-31			
29	4234.4482	0.4441	+41			
30	4235.9853					
31	4237.4479	0.4409	+70			

tainly too large. To resolve this difficulty a value of $\gamma_e = 1.0 \times 10^{-6}$ was adopted for calculations of the frequencies of all band lines. Using $B_0 = 1.922521$ and $\Delta B_{2-0} = -0.035008$, values of $B_e = 1.932174$ and $\alpha_e = -0.017507 \text{ cm}^{-1}$ result.

Using these constants $\Delta B_{3-1} = -0.035004$ and $\Delta B_{4-2} = -0.035000$ can be calculated. Using $H_0 = H_1 = H_2 = \dots = 5.8 \times 10^{-12}$ and $\Delta D_{2-0} = \Delta D_{3-1} = \Delta D_{4-2} = \dots = 1.9 \times 10^{-9} \text{ cm}^{-1}$ the band lines were calculated. The results are given in Tables III and IV along with the measured frequencies. The probable errors are ± 0.0043 and $\pm 0.0034 \text{ cm}^{-1}$, respectively.

DETERMINATION OF VIBRATIONAL CONSTANTS

The equation

$$G_v = \omega_e(v + \frac{1}{2}) + \omega_e x_e(v + \frac{1}{2})^2 + \omega_e y_e(v + \frac{1}{2})^3 \quad (2)$$

was used to determine the vibrational constants ω_e , $\omega_e x_e$, and $\omega_e y_e$ of the ground electronic state of CO. A consideration of the data dictated that the best values to be used in determining these constants were the origins of the 1-0 and 2-0 bands and the sum of the origins of the 3-1 and 4-2 bands. The results, in wave numbers, are $\omega_e = 2169.8232$, $\omega_e x_e = -13.2932$, and $\omega_e y_e = 0.01144$. Reverting to Eq. (2), the origins of various bands were computed, using these values. The calculated and measured results are given in Table V.

For a further verification of the accuracy of these band origins, the Ritz combination principle was employed, and its results were compared with the data from earlier independent investigations. These results are also given in Table V. It can be seen that the calculated values indicate excellent agreement with the observed frequencies. In addition the agreement of measured values with those obtained from the combination principle is clearly within the experimental errors.

TABLE V
CALCULATED AND OBSERVED BAND ORIGINS FOR SEVERAL BANDS OF CO

Band	Observed (Reference)	Calc (cm ⁻¹)	Ritz combination principle	Obs (cm ⁻¹)
1-0	7	2143.2740		2143.2740
2-0	7	4260.0646		4260.0646
3-1		4207.1664		4207.1680
4-2		4154.4056		4154.4040
5-3		4101.7820		
6-4		4049.2958		
7-5		3996.9466		
3-0	5	6350.4404	6350.4420	6350.436
4-0	1	8414.4702	8414.4686	8414.458

TABLE VI
COMPARISON OF CALCULATED VALUES OF THE 5-3, 6-4, AND 7-5 BANDS OF CO WITH THE MEASURED VALUES OF
GOLDBERG AND MUELLER ADJUSTED BY 0.05 CM⁻¹

5-3 Band $R(J)$				6-4 Band $R(J)$				7-5 Band $R(J)$			
J	Calc	G&M Obs	$C-O \times 10^2$	J	Calc	G&M Obs	$C-O \times 10^2$	J	Calc.	G&M Obs.	$C-O \times 10^2$
3	4116.0406	4116.05	+1	14	4096.3907	4096.44	-5	6	4020.6691	4020.57	+10
4	4119.4292	4119.43	0	19	4108.5044	4108.51	-1	12	4038.2355	4038.19	+4
12	4143.9793	4144.00	-2	24	4118.7956	4118.83	-3	13	4040.9125	4040.85	+6
15	4152.0034	4151.98	+2	27	4124.0879	4125.00	-1	16	4048.5108	4048.53	-2
20	4163.9282	4163.93	0	29	4127.2460	4127.23	+2	18	4053.2143	4053.17	+4
23	4170.2071	4170.29	-9	31	4130.1068	4130.08	+2	23	4063.6973	4063.73	-3
27	4177.5506	4177.59	-5	32	4131.4253	4131.43	0	31	4076.6420	4076.69	-5
29	4180.7782	4180.84	-6	36	4135.9491	4135.99	-4	32	4077.9258	4078.02	-9
33	4186.3401	4186.39	-6					37	4083.2203	4083.17	+5
$P(J)$											
11	4056.8248	4056.76	+6	3	4037.9714	4037.88	+9				
15	4038.4152	4038.36	+6								
23	3998.3515	3998.33	+2								

THE 5-3, 6-4, AND 7-5 BANDS

The molecular constants for these bands were calculated in order to predict the lines in these bands which were observed by Goldberg and Mueller (3). The results are as given below.

5-3 Band	6-4 Band	7-5 Band
$\nu_0 = 4101.7840$	$\nu_0 = 4049.2958$	$\nu_0 = 3996.9466$
$B_5 = 1.835010$	$B_6 = 1.817521$	$B_7 = 1.800026$
$D_5 = -6.1145 \times 10^{-6}$	$D_6 = -6.1136 \times 10^{-6}$	$D_7 = -6.1126 \times 10^{-6}$

The calculated lines are listed in Table VI. It was found that as good a fit could be obtained from the above constants as from the constants used by Goldberg and Mueller, provided 0.050 cm^{-1} is added to their measured frequencies. This difference is suspected to be a displacement error since a similar discrepancy was observed in the 2-0, 3-1, and 4-2 bands as well. The wavelengths of Reference 3 were converted to vacuum wave numbers through the Edlén dispersion formula (16). Table VI also lists the adjusted experimental results of Goldberg and Mueller.

DETERMINATION OF POTENTIAL CONSTANTS

From the values of ω_e , $\omega_e x_e$, $\omega_e y_e$, B_e , α_e , and γ_e , the first four potential constants of Dunham (12) were determined. The results are:

$$\begin{aligned} a_1 &= -2.6974, & a_3 &= -5.9589, \\ a_2 &= 4.5065, & a_4 &= 7.0457. \end{aligned}$$

These potential constants were then used to calculate the following values in wave numbers:

$$\begin{aligned} Y_{02} \sim D_e &= -6.1199 \times 10^{-6}, & Y_{03} \sim H_e &= +5.87 \times 10^{-12}, \\ Y_{12} \sim \beta_e &= +0.9833 \times 10^{-9}, & Y_{13} \sim \eta_e &= -1.4 \times 10^{-13}. \end{aligned}$$

It is clear that these values agree very well with the constants obtained by Rank *et al.* (5) which were the basis for calculating the frequencies of band lines given in Tables I, III, IV, and VI.

RECEIVED September 25, 1965

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