Rotational fine structure in the 0,0 and 0,1 bands of the O2(1Δg- 3Σg¯) system

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ROTATIONAL FINE STRUCTURE IN THE 0,0 AND 0,1 BANDS OF THE $O_2(^1\Delta_g - {}^3\Sigma_g^-)$ SYSTEM

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ABSTRACT

The observations of the 0,0 (1.27μ) and 0,1 (1.58μ) bands of the O_2 ($^1\Delta_g - {}^3\Sigma_g^-$) system arising from the airglow surrounding the earth have introduced the necessity for calculating the theoretical spectra of these two bands. All the necessary constants are available in the literature to a sufficient degree of accuracy, and the methods to be employed in calculating the spectra are well established. The wave-numbers in vacuum and wavelengths in air were calculated for all the important transitions in each band. The intensity of each rotational line was calculated for temperatures of 200°K, 250°K, and 300°K. The transitions were arranged in order of wavelength, and then plotted after a triangular transmission function typical of a scanning grating spectrometer was applied.

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ROTATIONAL FINE STRUCTURE IN THE 0,0 AND 0,1 BANDS OF THE $O_2(^1\Delta_g - {}^3\Sigma_g^-)$ SYSTEM

– R.L. Gattinger –

INTRODUCTION

The $O_2(^1\Delta_g - {}^3\Sigma_g^-)$ infrared atmospheric oxygen system, which originates in the airglow surrounding the earth, plays an important role in the photochemistry of the atmosphere. The observations of the 0,0 (1.27 μ) and 0,1 (1.58 μ) bands of this system have been reviewed recently by several authors (Hunten 1967; Evans 1967; Noxon 1968; Gattinger 1968). Both bands are emitted continually with the brightness of the 0,0 band being about 25 MR at local noon and about 100 kR during the late night hours. The 0,1 band is about 50 times weaker, but it is usually selected for ground-based observations because the 0,0 band is strongly absorbed by the $O_2(^3\Sigma_g^-)$ molecules in the lower atmosphere. The $O_2(^1\Delta_g)$ state has a lifetime of about 45 minutes, and this makes it possible to observe the emissions in the evening twilight airglow more readily than at dawn if there is an appreciable amount of scattered solar radiation in the field of view of the instrument.

The existence of the $O_2(^1\Delta_g)$ state was suggested by Ellis and Kneser (1933) on the basis of the absorption spectrum of liquid oxygen, and also on the atmospheric absorption in the solar spectrum. The $O_2(^1\Delta_g - {}^3\Sigma_g^-)$ system was positively identified by Herzberg (1934) in a terrestrial solar spectrum which included the 0,0 band at 1.27 μ. A more accurate analysis of the $O_2(^1\Delta_g - {}^3\Sigma_g^-)$ system was presented by Herzberg and Herzberg (1947); they derived the required molecular constants of the $O_2(^1\Delta_g)$ state to an accuracy which is sufficient for the present analysis.

An accurate set of molecular constants for the $O_2(^3\Sigma_g^-)$ state was determined by Babcock and Herzberg (1948) from spectra of the $O_2(^1\Sigma_g^+ - {}^3\Sigma_g^-)$ system, commonly known as the atmospheric oxygen system.

The formulas required to calculate the wavenumbers in vacuum, wavelengths in air, and the relative intensities of the rotational lines in each band are readily available and will be discussed in the following sections. A digital computer program was written in the Fortran language to solve the necessary equations.

CALCULATION OF THE ENERGY LEVELS IN THE $O_2(^3\Sigma_g^-)$ STATE

The contents of this section are based largely upon the results obtained by Babcock and Herzberg (1948). The fine structure of the $O_2(^3\Sigma_g^-)$ state is shown in Fig. 1. The rotational levels with even values of K'' are absent, and those with odd values of K'' are split into three levels, $F_1''(K)$, $F_2''(K)$, and $F_3''(K)$, corresponding to the cases where $J'' = K'' + 1$, $J'' = K''$, and $J'' = K'' - 1$, respectively. The formulas for these levels in a $^3\Sigma$ state are as follows (Babcock and Herzberg 1948):

$$F_2''(K) = B_v K''(K''+1) - D_v K''^2 (K''+1)^2 \qquad (1)$$

$$F_1''(K) = F_2''(K) + (2K''+3)B_v - \lambda_v - [(2K''+3)^2 B_v^2 + \lambda_v^2 - 2\lambda_v B_v]^{1/2} + \gamma(K''+1) \qquad (2)$$

$$F_3''(K) = F_2''(K) - (2K''-1)B_v - \lambda_v + [(2K''-1)^2 B_v^2 + \lambda_v^2 - 2\lambda_v B_v]^{1/2} - \gamma K''. \qquad (3)$$

The constants required to evaluate these expressions are given in Table I. The rotational energy levels are referred to the non-existent $F_2''(0)$ state in the vibrational energy level concerned.

The energy separation, $\Delta G_{1/2}$, between the two lowest vibrational levels is also given in Table I. It is of interest to note that Harrison (1957) used a value of 1556.2153 cm^{-1} which was derived using the formula (Herzberg (1950); formula III, 81)

$$\Delta G_{1/2} = \omega_e - 2\omega_e x_e \qquad (4)$$

However, the formula (Herzberg (1950); formula III, 81*a*)

$$\Delta G_{1/2} = \omega_e - 2\omega_e x_e + 3.25\ \omega_e y_e + 5\omega_e z_e \qquad (5)$$

must be used to obtain the value of $\Delta G_{1/2}$ given in Table I.

The energy of the non-existent $F_2''(0)$ state in the lowest vibrational level of the $O_2(^3\Sigma_g^-)$ state was set equal to zero, and all other levels were referred to this state; the

Table I

Vibrational and rotational constants of the $O_2(^3\Sigma_g^-)$ and $O_2(^1\Delta_g)$ states

Constant	$^3\Sigma_g^-$ (cm^{-1})	$^1\Delta_g$ (cm^{-1})
$\Delta G_{1/2}$	1556.3856	
$A_0 = \nu_{00}$		7882.39
ω_e	1580.3613	
$\omega_e x_e$	12.0730	
$\omega_e y_e$	0.0546	
$\omega_e z_e$	-0.00143	
B_0	1.437770	1.41783
B_1	1.421979	
D_0	4.913×10^{-6}	4.86×10^{-6}
D_1	4.825×10^{-6}	
λ_0	1.984	
λ_1	1.993	
γ	-0.00837	

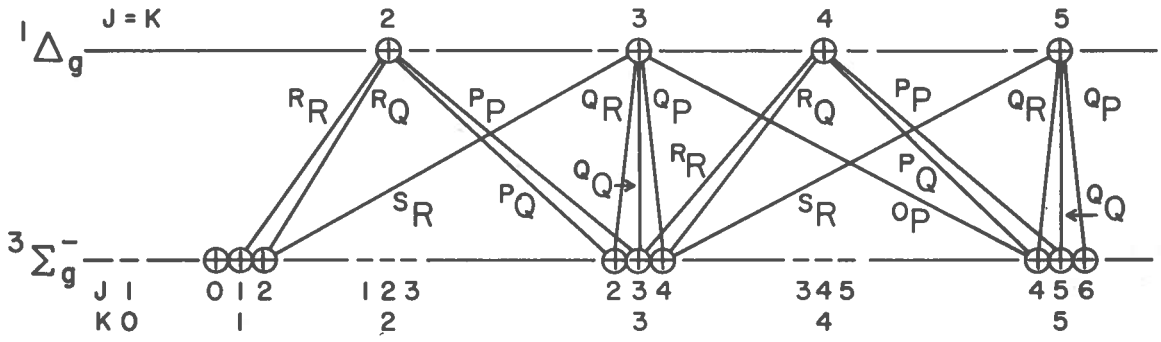

Fig. 1 Sample of allowed (circled) energy levels and transitions in the $O_2(^1\Delta_g - {}^3\Sigma_g^-)$ system. The rotational transition scheme is identical for the 0,0 and 0,1 bands.

quantity $\Delta G_{½}$ was added to each of the rotational energy levels calculated for the state $v'' = 1$ to make this condition true for both vibrational levels. The energy levels are listed in Table II.

CALCULATION OF THE ENERGY LEVELS IN THE $O_2(^1\Delta_g)$ STATE

The results of Herzberg and Herzberg (1947) were used to calculate the energy levels in the $O_2(^1\Delta_g)$ state. The rotational fine structure of this state is shown in Fig. 1. In a singlet state, $J' = K'$, since the spin, $S = 0$; also, in a Δ state the levels, $J' = 0$ and $J' = 1$, are absent. Only the positive rotational levels occur, and in these calculations the λ doubling has been ignored. The formula for the calculation of the rotational energy levels is (Herzberg (1950); formula III, 104)

$$F'(J) = B_v J'(J' + 1) - D_v J'^2 (J' + 1)^2 \qquad (6)$$

which refers the levels to the non-existent $F'(0)$ level. These $O_2(^1\Delta_g)$ levels were referred to the non-existent $O_2(^3\Sigma_g^-)$, $v'' = 0$, $F_2''(0)$ level by adding the term, ν_{00}, for the $O_2(^1\Delta_g - {}^3\Sigma_g^-)$ system to each of the rotational levels in the $O_2(^1\Delta_g)$ state. The constants required for these calculations are given in Table I, and the calculated energy levels are given in Table III.

CALCULATION OF THE WAVENUMBERS AND WAVELENGTHS OF THE TRANSITIONS IN THE 0,0 AND 0,1 BANDS

Examples of the types of transitions which occur in the $O_2(^1\Delta_g - {}^3\Sigma_g^-)$ system (Herzberg and Herzberg(1947)) are shown in Fig. 1. Each band contains nine branches, and the changes in the quantum numbers, J and K, corresponding to each branch are given in Table IV. The wavenumbers in vacuum of the transitions in each branch of the two bands, calculated by determining the difference in energy between the upper and lower levels involved, are given in Table V.

The wavelengths in air, also given in Table V, were calculated with the formula for the refractive index of air given by Coleman, Bozman, and Meggers (1960); page 4,

$$n = 1 + 6432.8 \times 10^{-8} + \frac{2949810}{146 \times 10^8 - \sigma^2} + \frac{25540}{41 \times 10^8 - \sigma^2} \qquad (7)$$

where σ is the vacuum wavenumber.

The good agreement between the results given in Table V and those given by Herzberg and Herzberg (1947) and Mohler (1955) indicates that the methods employed are correct.

Table II

Energy levels in the $O_2(^3\Sigma_g^-)$ state in the two lowest vibrational levels

	SIGMA STATE V = 0		
K	F1(K)	F2(K)	F3(K)
1	0.9989	2.8755	0.0083
3	15.3036	17.2525	15.1695
5	41.1418	43.1287	41.1179
7	78.4849	80.4997	78.5269
9	127.3211	129.3595	127.4146
11	187.6402	189.7000	187.7787
13	259.4307	261.5110	259.6108
15	342.6816	344.7815	342.9016
17	437.3784	439.4971	437.6362
19	543.5063	545.6431	543.8010
21	661.0457	663.2007	661.3767
23	789.9790	792.1516	790.3459
25	930.2839	932.4744	930.6865
27	1081.9377	1084.1455	1082.3752
29	1244.9153	1247.1406	1245.3882
31	1419.1899	1421.4329	1419.6975
33	1604.7322	1606.9922	1605.2744
35	1801.5125	1803.7898	1802.0891
37	2009.4973	2011.7917	2010.1084
39	2228.6523	2230.9641	2229.2981
41	2458.9421	2461.2710	2459.6221
43	2700.3276	2702.6733	2701.0417
45	2952.7683	2955.1311	2953.5161
47	3216.2239	3218.6038	3217.0061
49	3490.6482	3493.0452	3491.4644
51	3775.9983	3778.4119	3776.8481
53	4072.2195	4074.6521	4073.1052

	SIGMA STATE V = 1		
K	F1(K)	F2(K)	F3(K)
1	1557.3394	1559.2292	1556.3931
3	1571.4878	1573.4485	1571.3596
5	1597.0425	1599.0403	1597.0222
7	1633.9756	1636.0010	1634.0200
9	1682.2756	1684.3245	1682.3711
11	1741.9324	1744.0024	1742.0728
13	1812.9358	1815.0256	1813.1169
15	1895.2732	1897.3823	1895.4939
17	1988.9307	1991.0588	1989.1895
19	2093.8943	2096.0405	2094.1899
21	2210.1453	2212.3096	2210.4771
23	2337.6653	2339.8474	2338.0330
25	2476.4331	2478.6331	2476.8367
27	2626.4260	2628.6433	2626.8645
29	2787.6199	2789.8547	2788.0935
31	2959.9880	2962.2402	2960.4963
33	3143.5020	3145.7712	3144.0447
35	3338.1318	3340.4185	3338.7090
37	3543.8457	3546.1494	3544.4573
39	3760.6089	3762.9299	3761.2551
41	3988.3811	3990.7253	3989.0676
43	4227.1328	4229.4961	4227.8477
45	4476.8242	4479.2031	4477.5703
47	4737.4180	4739.8125	4738.1953
49	5008.8516	5011.2695	5009.6680
51	5291.1016	5293.5352	5291.9570
53	5584.1172	5586.5664	5585.0039

Table III

Energy levels in the $O_2(^1\Delta_g)$, $v' = 0$ state

DELTA K	STATE V = 0 F(K)		
2	7890.89	28	9030.46
3	7899.40	29	9112.22
4	7910.74	30	9196.76
5	7924.91	31	9284.09
6	7941.93	32	9374.19
7	7961.77	33	9467.07
8	7984.44	34	9562.72
9	8009.95	35	9661.13
10	8038.29	36	9762.31
11	8069.45	37	9866.25
12	8103.45	38	9972.93
13	8140.27	39	10082.37
14	8179.91	40	10194.55
15	8222.38	41	10309.48
16	8267.68	42	10427.13
17	8315.79	43	10547.52
18	8366.71	44	10670.63
19	8420.46	45	10796.47
20	8477.02	46	10925.02
21	8536.38	47	11056.27
22	8598.56	48	11190.23
23	8663.55	49	11326.89
24	8731.33	50	11466.25
25	8801.92	51	11608.29
26	8875.30	52	11753.01
27	8951.48	53	11900.40
		54	12050.47

Table IV

Changes in the quantum numbers J and K for the nine branches in each band of the $O_2(^1\Delta_g - {}^3\Sigma_g^-)$ system

$J' - J''$ \ $K' - K''$	-2	-1	0	+1	+2
-1	${}^{O}P$	${}^{P}P$	${}^{Q}P$		
0		${}^{P}Q$	${}^{Q}Q$	${}^{R}Q$	
+1			${}^{Q}R$	${}^{R}R$	${}^{S}R$

Table Va

Wavenumbers (vacuum) and wavelengths (air) of the transitions in the 0,0 band of the $O_2(^1\Delta_g - {}^3\Sigma_g^-)$ system

0-0 BAND

J	RR	RQ	PP	PQ
2	7888.01	7889.89	7873.64	7875.72
2	12674.02	12671.00	12697.16	12693.80
4	7893.48	7895.43	7867.61	7869.62
4	12665.23	12662.11	12706.88	12703.64
6	7898.80	7900.78	7861.43	7863.40
6	12656.71	12653.53	12716.88	12713.69
8	7903.94	7905.95	7855.08	7857.02
8	12648.48	12645.25	12727.15	12724.00
10	7908.93	7910.96	7848.59	7850.51
10	12640.50	12637.25	12737.68	12734.57
12	7913.75	7915.81	7841.94	7843.84
12	12632.80	12629.51	12748.48	12745.39
14	7918.40	7920.48	7835.13	7837.01
14	12625.37	12622.06	12759.56	12756.50
16	7922.89	7924.99	7828.18	7830.04
16	12618.22	12614.87	12770.89	12767.86
18	7927.21	7929.34	7821.07	7822.91
18	12611.34	12607.96	12782.50	12779.49
20	7931.37	7933.51	7813.81	7815.64
20	12604.73	12601.34	12794.37	12791.38
22	7935.36	7937.52	7806.41	7808.21
22	12598.39	12594.97	12806.50	12803.54
24	7939.18	7941.35	7798.86	7800.64
24	12592.34	12588.89	12818.91	12815.97
26	7942.83	7945.02	7791.16	7792.93
26	12586.55	12583.08	12831.57	12828.66
28	7946.31	7948.52	7783.32	7785.07
28	12581.04	12577.54	12844.50	12841.61
30	7949.62	7951.84	7775.33	7777.06
30	12575.80	12572.28	12857.70	12854.83
32	7952.76	7955.00	7767.20	7768.91
32	12570.84	12567.29	12871.15	12868.31
34	7955.73	7957.98	7758.93	7760.63
34	12566.14	12562.58	12884.88	12882.05
36	7958.52	7960.80	7750.52	7752.20
36	12561.73	12558.14	12898.85	12896.05
38	7961.14	7963.43	7741.97	7743.63
38	12557.60	12553.98	12913.10	12910.32
40	7963.59	7965.90	7733.28	7734.93
40	12553.73	12550.09	12927.61	12924.85
42	7965.86	7968.19	7724.46	7726.09
42	12550.16	12546.49	12942.37	12939.64
44	7967.96	7970.30	7715.50	7717.11
44	12546.86	12543.16	12957.40	12954.69
46	7969.88	7972.25	7706.41	7708.01
46	12543.82	12540.11	12972.68	12969.99
48	7971.63	7974.01	7697.19	7698.77
48	12541.07	12537.34	12988.23	12985.55
50	7973.20	7975.60	7687.83	7689.39
50	12538.61	12534.84	13004.03	13001.39
52	7974.59	7977.01	7678.36	7679.90
52	12536.41	12532.62	13020.08	13017.46

Table Va continued

J	QR	QQ	QP	OP	SR
3	7884.23	7882.14	7884.09	7858.28	7898.40
3	12680.10	12683.45	12680.32	12721.97	12657.35
5	7883.79	7881.79	7883.77	7846.39	7909.61
5	12680.80	12684.03	12680.84	12741.25	12639.41
7	7883.24	7881.27	7883.28	7834.35	7920.62
7	12681.69	12684.86	12681.62	12760.82	12621.83
9	7882.53	7880.59	7882.62	7822.17	7931.46
9	12682.83	12685.95	12682.68	12780.70	12604.59
11	7881.67	7879.75	7881.81	7809.84	7942.13
11	12684.21	12687.30	12683.98	12800.88	12587.66
13	7880.66	7878.76	7880.84	7797.37	7952.63
13	12685.85	12688.90	12685.56	12821.36	12571.04
15	7879.48	7877.60	7879.70	7784.75	7962.95
15	12687.74	12690.77	12687.39	12842.14	12554.75
17	7878.15	7876.29	7878.41	7771.98	7973.10
17	12689.89	12692.89	12689.47	12863.23	12538.76
19	7876.65	7874.81	7876.95	7759.08	7983.08
19	12692.30	12695.26	12691.82	12884.62	12523.09
21	7875.00	7873.18	7875.34	7746.04	7992.87
21	12694.95	12697.89	12694.42	12906.32	12507.74
23	7873.20	7871.39	7873.57	7732.86	8002.50
23	12697.86	12700.77	12697.27	12928.31	12492.70
25	7871.23	7869.45	7871.64	7719.54	8011.94
25	12701.03	12703.92	12700.38	12950.61	12477.97
27	7869.11	7867.34	7869.54	7706.09	8021.20
27	12704.47	12707.32	12703.76	12973.21	12463.57
29	7866.83	7865.08	7867.30	7692.52	8030.28
29	12708.14	12710.97	12707.38	12996.11	12449.48
31	7864.39	7862.66	7864.90	7678.81	8039.17
31	12712.09	12714.89	12711.26	13019.30	12435.71
33	7861.79	7860.08	7862.34	7664.98	8047.88
33	12716.29	12719.06	12715.41	13042.80	12422.25
35	7859.04	7857.34	7859.62	7651.02	8056.40
35	12720.73	12723.49	12719.80	13066.59	12409.12
37	7856.14	7854.45	7856.75	7636.95	8064.73
37	12725.44	12728.17	12724.45	13090.68	12396.30
39	7853.07	7851.41	7853.72	7622.75	8072.87
39	12730.41	12733.11	12729.36	13115.06	12383.80
41	7849.85	7848.20	7850.53	7608.43	8080.82
41	12735.63	12738.30	12734.53	13139.73	12371.61
43	7846.48	7844.84	7847.19	7594.00	8088.57
43	12741.11	12743.76	12739.95	13164.71	12359.76
45	7842.95	7841.34	7843.70	7579.46	8096.14
45	12746.84	12749.46	12745.62	13189.96	12348.20
47	7839.27	7837.67	7840.05	7564.81	8103.50
47	12752.83	12755.43	12751.55	13215.51	12336.98
49	7835.43	7833.85	7836.25	7550.04	8110.67
49	12759.07	12761.65	12757.74	13241.36	12326.09
51	7831.44	7829.87	7832.29	7535.18	8117.64
51	12765.57	12768.12	12764.19	13267.46	12315.50

Table Vb

Wavenumbers (vacuum) and wavelengths (air) of the transitions in the 0,1 band of the O_2 ($^1\Delta_g - {}^3\Sigma_g^-$) system

0-1 BAND

J	RR	RQ	PP	PQ
2	6331.66	6333.55	6317.44	6319.53
2	15789.35	15784.64	15824.89	15819.66
4	6337.29	6339.25	6311.70	6313.71
4	15775.33	15770.45	15839.30	15834.23
6	6342.88	6344.88	6305.92	6307.90
6	15761.41	15756.45	15853.80	15848.82
8	6348.44	6350.46	6300.11	6302.07
8	15747.62	15742.60	15868.41	15863.49
10	6353.96	6356.01	6294.29	6296.21
10	15733.93	15728.86	15883.11	15878.24
12	6359.45	6361.52	6288.42	6290.33
12	15720.36	15715.25	15897.91	15893.09
14	6364.89	6366.98	6282.53	6284.42
14	15706.93	15701.77	15912.82	15908.05
16	6370.29	6372.40	6276.61	6278.48
16	15693.59	15688.40	15927.83	15923.08
18	6375.65	6377.78	6270.67	6272.52
18	15680.40	15675.17	15942.92	15938.21
20	6380.97	6383.12	6264.70	6266.54
20	15667.33	15662.06	15958.11	15953.44
22	6386.25	6388.41	6258.71	6260.53
22	15654.38	15649.08	15973.37	15968.75
24	6391.48	6393.66	6252.70	6254.49
24	15641.56	15636.23	15988.75	15984.16
26	6396.67	6398.87	6246.66	6248.44
26	15628.89	15623.51	16004.20	15999.65
28	6401.81	6404.03	6240.60	6242.36
28	15616.33	15610.93	16019.74	16015.22
30	6406.91	6409.14	6234.52	6236.26
30	15603.91	15598.47	16035.37	16030.89
32	6411.95	6414.20	6228.42	6230.14
32	15591.64	15586.16	16051.08	16046.62
34	6416.95	6419.21	6222.30	6224.01
34	15579.50	15573.99	16066.87	16062.45
36	6421.89	6424.18	6216.16	6217.85
36	15567.50	15561.96	16082.73	16078.35
38	6426.78	6429.09	6210.00	6211.68
38	15555.66	15550.08	16098.68	16094.34
40	6431.62	6433.95	6203.83	6205.48
40	15543.95	15538.34	16114.70	16110.39
42	6436.41	6438.75	6197.64	6199.29
42	15532.39	15526.74	16130.80	16126.50
44	6441.14	6443.50	6191.43	6193.06
44	15520.99	15515.30	16146.96	16142.71
46	6445.81	6448.19	6185.20	6186.82
46	15509.73	15504.01	16163.22	16159.00
48	6450.42	6452.82	6178.96	6180.57
48	15498.64	15492.89	16179.54	16175.35
50	6454.98	6457.39	6172.71	6174.29
50	15487.71	15481.91	16195.93	16191.79
52	6459.47	6461.91	6166.44	6168.00
52	15476.93	15471.10	16212.40	16208.29

Table Vb continued

J	QR	QQ	QP	OP	SR
3	6328.04	6325.95	6327.91	6302.37	6342.06
3	15798.40	15803.61	15798.71	15862.72	15763.46
5	6327.89	6325.87	6327.87	6290.89	6353.43
5	15798.76	15803.80	15798.80	15891.68	15735.26
7	6327.75	6325.77	6327.79	6279.40	6364.73
7	15799.12	15804.07	15799.00	15920.76	15707.32
9	6327.58	6325.62	6327.67	6267.87	6375.97
9	15799.54	15804.43	15799.30	15950.03	15679.62
11	6327.38	6325.45	6327.52	6256.34	6387.18
11	15800.04	15804.86	15799.68	15979.45	15652.11
13	6327.15	6325.24	6327.33	6244.77	6398.34
13	15800.60	15805.37	15800.15	16009.04	15624.81
15	6326.89	6325.00	6327.11	6233.19	6409.45
15	15801.26	15805.98	15800.71	16038.79	15597.73
17	6326.59	6324.72	6326.85	6221.59	6420.51
17	15802.00	15806.67	15801.35	16068.68	15570.85
19	6326.27	6324.41	6326.56	6209.98	6431.52
19	15802.82	15807.44	15802.07	16098.74	15544.19
21	6325.90	6324.07	6326.23	6198.35	6442.49
21	15803.72	15808.30	15802.89	16128.95	15517.73
23	6325.51	6323.70	6325.88	6186.71	6453.40
23	15804.70	15809.23	15803.78	16159.29	15491.50
25	6325.08	6323.29	6325.49	6175.05	6464.25
25	15805.77	15810.26	15804.76	16189.79	15465.48
27	6324.62	6322.84	6325.05	6163.39	6475.05
27	15806.93	15811.38	15805.84	16220.43	15439.70
29	6324.12	6322.36	6324.60	6151.72	6485.79
29	15808.16	15812.57	15806.98	16251.20	15414.13
31	6323.59	6321.85	6324.10	6140.04	6496.47
31	15809.50	15813.86	15808.22	16282.10	15388.79
33	6323.02	6321.30	6323.57	6128.36	6507.08
33	15810.92	15815.24	15809.56	16313.14	15363.69
35	6322.42	6320.71	6323.00	6116.67	6517.63
35	15812.42	15816.70	15810.98	16344.32	15338.83
37	6321.79	6320.09	6322.40	6104.99	6528.11
37	15814.02	15818.25	15812.48	16375.59	15314.20
39	6321.11	6319.44	6321.76	6093.30	6538.52
39	15815.70	15819.89	15814.07	16407.00	15289.82
41	6320.41	6318.75	6321.09	6081.63	6548.87
41	15817.46	15821.61	15815.75	16438.49	15265.66
43	6319.67	6318.02	6320.39	6069.95	6559.14
43	15819.30	15823.43	15817.52	16470.12	15241.76
45	6318.90	6317.27	6319.64	6058.27	6569.34
45	15821.24	15825.33	15819.37	16501.86	15218.10
47	6318.08	6316.46	6318.86	6046.61	6579.45
47	15823.29	15827.34	15821.35	16533.71	15194.71
49	6317.23	6315.62	6318.04	6034.94	6589.48
49	15825.43	15829.44	15823.38	16565.67	15171.59
51	6316.33	6314.75	6317.19	6023.29	6599.44
51	15827.67	15831.62	15825.52	16597.72	15148.69

CALCULATION OF THE RELATIVE INTENSITIES OF THE TRANSITIONS IN EACH BAND

The intensity of an emission line in units of energy is given by Herzberg (1950); formula I, 46,

$$I_{J'J''} = N_{J'} \; hc\nu_{J'J''} \; A_{J'J''} \, , \tag{8}$$

where $N_{J'}$ is the population in the upper state and $A_{J'J''}$ is the Einstein transition probability of spontaneous emission.

The relative populations of the rotational levels in the $O_2(^1\Delta_g)$ state were calculated using the simplified relationship (Herzberg (1950); formula III, 161)

$$N_{J'} = (2J' + 1) \exp[- (F' (J) - \nu_{00}) \, hc/kT] \tag{9}$$

where the energy levels are referred to the non-existent $F'(0)$ state. The relative populations obtained for various temperatures are given in Table VI.

The expression for $A_{J'J''}$ (Herzberg (1950); formula I, 54; also page 127) was approximated by

$$A_{J'J''} \propto \frac{\nu^3_{J'J''} \; S_J}{2J' + 1} \tag{10}$$

The line strength values, S_J, are given in Table VII (Van Vleck (1934)).

The relative intensities of the rotational lines given in Table VIII in photon units and at various temperatures were calculated using the expression

$$I_{J'J''} = CN_{J'} \; \nu^3_{J'J''} \quad \frac{S_J}{2J' + 1} \, , \tag{11}$$

where C was chosen so that the results would be in a convenient range.

SMEARING AND PLOTTING OF SPECTRA

All the transitions in each band were arranged in wavelength order within the computer program to facilitate the convolution with an instrumental smearing function, and also to plot the resultant spectrum. To simplify the Fortran coding required to do this, the wavelengths were rounded to the nearest ¼ Å; this introduced a maximum wavelength error of 1/8 Å. A triangular smearing function typical of a scanning grating spectrometer with a given spectral slit width was applied to each spectrum by the Fortran program, and the spectra were then automatically plotted on a digital plotter.

The spectra in Figs. 2 and 3 were calculated for a temperature of 250°K, and for a triangular smearing function of 2 Å full width at half-height. Figure 3 shows the central portion of each band on an expanded scale.

The spectra in Fig. 4 correspond to a temperature of 300°K with a 10-Å triangular smearing function. The 10 Å on either end of each band were not plotted because only those transitions occurring within a 500-Å interval were considered when smearing the spectrum. The spectral shape is very similar to that derived by Gush and Buijs (1964).

A temperature of 200°K and a 50-Å smearing function were used to derive the spectra in Fig. 5. Here again the 50 Å on either end of each band were not plotted since this would require information on transitions outside the 500-Å range assumed for the smearing function.

DIGITAL COMPUTER PROGRAM

A simplified flow chart of the program is given in Fig. 6. The time required to compile and execute the program for one temperature and one band pair is approximately 3 minutes. The plotting of the spectra on an off-line digital plotter requires from 10 to 20 minutes per band pair depending upon the number of points to be plotted.

SUMMARY

The theoretical spectra of the 0,0 and 0,1 bands of the $O_2(^1\Delta_g - {}^3\Sigma_g^-)$ system have been calculated to aid in the analysis of the observations of these emissions. A positive identification of the observed emissions is made possible by a direct comparison between the observed and theoretical spectra. Also, if the instrument used to make the observations does not exhibit a linear response at all wavelengths, the observed brightness may be corrected in accordance with the theoretical spectral information so that the total band brightness and possibly the true band shape may be derived. The theoretical results in this report have been presented in various forms to facilitate the comparison between the experimental and theoretical spectra.

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Table VI

Relative populations in the rotational levels of the $O_2(^1\Delta_g)$, $v' = 0$ state at various temperatures

J	TEMP = 200.0°K POPULATION	J	TEMP = 250.0°K POPULATION
2	4.70327	2	4.76118
3	6.19365	3	6.34712
4	7.33941	4	7.64499
5	8.10066	5	8.61182
6	8.47070	6	9.22835
7	8.47359	7	9.49888
8	8.15810	8	9.44846
9	7.58922	9	9.11819
10	6.84097	10	8.56127
11	5.98767	11	7.83704
12	5.09627	12	7.00471
13	4.22313	13	6.12041
14	3.41039	14	5.23266
15	2.68583	15	4.38061
16	2.06403	16	3.59316
17	1.54867	17	2.88922
18	1.13492	18	2.27831
19	0.81268	19	1.76257
20	0.56875	20	1.33813
21	0.38915	21	0.99722
22	0.26037	22	0.72965
23	0.17039	23	0.52429
24	0.10908	24	0.37003
25	0.06832	25	0.25655
26	0.04188	26	0.17477
27	0.02512	27	0.11699
28	0.01475	28	0.07696
29	0.00848	29	0.04976
30	0.00477	30	0.03162
31	0.00263	31	0.01976
32	0.00142	32	0.01214
33	0.00075	33	0.00733
34	0.00039	34	0.00435
35	0.00020	35	0.00254
36	0.00010	36	0.00146
37	0.00005	37	0.00082
38	0.00002	38	0.00046
39	0.00001	39	0.00025
40	0.00000	40	0.00013
41	0.00000	41	0.00007
42	0.00000	42	0.00004
43	0.00000	43	0.00002
44	0.00000	44	0.00001
45	0.00000	45	0.00000
46	0.00000	46	0.00000
47	0.00000	47	0.00000
48	0.00000	48	0.00000
49	0.00000	49	0.00000
50	0.00000	50	0.00000
51	0.00000	51	0.00000
52	0.00000	52	0.00000
53	0.00000	53	0.00000
54	0.00000	54	0.00000
55	0.00000	55	0.00000

Table VI (continued) TEMP = 300.0°K

J	POPULATION		
		29	0.16188
2	4.80017	30	0.11158
3	6.45155	31	0.07580
4	7.85576	32	0.05077
5	8.97038	33	0.03352
6	9.77074	34	0.02182
7	10.25043	35	0.01400
8	10.42019	36	0.00886
9	10.30503	37	0.00553
10	9.94226	38	0.00340
11	9.37737	39	0.00207
12	8.65928	40	0.00124
13	7.83811	41	0.00073
14	6.96096	42	0.00043
15	6.06978	43	0.00024
16	5.19975	44	0.00014
17	4.37853	45	0.00008
18	3.62559	46	0.00004
19	2.95325	47	0.00002
20	2.36707	48	0.00001
21	1.86740	49	0.00001
22	1.45033	50	0.00000
23	1.10916	51	0.00000
24	0.83541	52	0.00000
25	0.61978	53	0.00000
26	0.45299	54	0.00000
27	0.32621	55	0.00000
28	0.23148		

Table VII

Line strengths of the nine branches in each band as a function of the quantum numbers in the $O_2(^1\Delta_g)$ state

$J' - J''$ \ $K' - K''$	-2	-1	0	+1	+2
-1	$\frac{(J'-1)\,J'}{2J'+3}$	$\frac{(J'-1)\,J'}{J'+1}$	$\frac{(J'-1)\,J'\,(J'+2)}{(J'+1)\,(2J'+3)}$		
0		$\frac{(J'+2)\,(J'-1)}{J'+1}$	$\frac{(J'+2)\,(J'-1)\,(2J'+1)}{J'\,(J'+1)}$	$\frac{(J'+2)\,(J'-1)}{J'}$	
+1			$\frac{(J'-1)\,(J'+1)\,(J'+2)}{J'\,(2J'-1)}$	$\frac{(J'+1)\,(J'+2)}{J'}$	$\frac{(J'+1)\,(J'+2)}{2J'-1}$

Table VIII

Relative intensities of rotational lines in the 0,0 and 0,1 bands of the $O_2(^1\Delta_g - {}^3\Sigma_g^-)$ system at various temperatures

0,0 BAND TEMP 200°K

J	RR	RQ	PP	PQ
2	8.0759	2.6939	0.8924	1.7863
4	8.7698	5.2658	2.7788	4.1714
6	8.7378	6.2460	3.9556	5.2781
8	7.7719	6.0495	4.2193	5.2781
10	6.2020	5.0783	3.7569	4.5116
12	4.4674	3.7831	2.9102	3.3977
14	2.9181	2.5310	2.0009	2.2884
16	1.7344	1.5316	1.2350	1.3903
18	0.9405	0.8421	0.6890	0.7661
20	0.4661	0.4221	0.3491	0.3843
22	0.2115	0.1933	0.1612	0.1760
24	0.0880	0.0810	0.0680	0.0737
26	0.0336	0.0311	0.0262	0.0283
28	0.0118	0.0110	0.0093	0.0099
30	0.0038	0.0035	0.0030	0.0032
32	0.0011	0.0011	0.0009	0.0010
34	0.0003	0.0003	0.0002	0.0003
36	0.0001	0.0001	0.0001	0.0001
38	0.0000	0.0000	0.0000	0.0000
40	0.0000	0.0000	0.0000	0.0000
42	0.0000	0.0000	0.0000	0.0000
44	0.0000	0.0000	0.0000	0.0000
46	0.0000	0.0000	0.0000	0.0000
48	0.0000	0.0000	0.0000	0.0000
50	0.0000	0.0000	0.0000	0.0000
52	0.0000	0.0000	0.0000	0.0000

J	QR	QQ	QP	OP	SR
3	3.3713	7.3689	1.0535	0.8345	5.0843
5	3.9277	10.7928	1.8883	1.5956	4.9580
7	3.8303	11.6618	2.2426	1.9565	4.5326
9	3.2805	10.5881	2.1511	1.9109	3.7597
11	2.5096	8.4114	1.7714	1.5908	2.8246
13	1.7305	5.9554	1.2864	1.1629	1.9266
15	1.0817	3.7960	0.8356	0.7583	1.1962
17	0.6152	2.1917	0.4895	0.4452	0.6776
19	0.3193	1.1509	0.2601	0.2367	0.3508
21	0.1515	0.5513	0.1258	0.1145	0.1663
23	0.0658	0.2414	0.0555	0.0505	0.0722
25	0.0262	0.0968	0.0224	0.0203	0.0288
27	0.0096	0.0356	0.0083	0.0075	0.0105
29	0.0032	0.0120	0.0028	0.0025	0.0035
31	0.0010	0.0037	0.0009	0.0008	0.0011
33	0.0003	0.0011	0.0002	0.0002	0.0003
35	0.0001	0.0003	0.0001	0.0001	0.0001
37	0.0000	0.0001	0.0000	0.0000	0.0000
39	0.0000	0.0000	0.0000	0.0000	0.0000
41	0.0000	0.0000	0.0000	0.0000	0.0000
43	0.0000	0.0000	0.0000	0.0000	0.0000
45	0.0000	0.0000	0.0000	0.0000	0.0000
47	0.0000	0.0000	0.0000	0.0000	0.0000
49	0.0000	0.0000	0.0000	0.0000	0.0000
51	0.0000	0.0000	0.0000	0.0000	0.0000

0,1 BAND TEMP 200°K

J	RR	RQ	PP	PQ
2	4.1768	1.3935	0.4610	0.9228
4	4.5383	2.7255	1.4347	2.1542
6	4.5246	3.2349	2.0415	2.7246
8	4.0272	3.1352	2.1769	2.7236
10	3.2160	2.6338	1.9377	2.3274
12	2.3183	1.9635	1.5006	1.7523
14	1.5155	1.3148	1.0316	1.1800
16	0.9015	0.7963	0.6366	0.7168
18	0.4893	0.4382	0.3551	0.3949
20	0.2427	0.2198	0.1799	0.1981
22	0.1102	0.1008	0.0831	0.0907
24	0.0459	0.0423	0.0350	0.0380
26	0.0175	0.0163	0.0135	0.0146
28	0.0062	0.0057	0.0048	0.0051
30	0.0020	0.0019	0.0016	0.0017
32	0.0006	0.0006	0.0005	0.0005
34	0.0002	0.0002	0.0001	0.0001
36	0.0000	0.0000	0.0000	0.0000
38	0.0000	0.0000	0.0000	0.0000
40	0.0000	0.0000	0.0000	0.0000
42	0.0000	0.0000	0.0000	0.0000
44	0.0000	0.0000	0.0000	0.0000
46	0.0000	0.0000	0.0000	0.0000
48	0.0000	0.0000	0.0000	0.0000
50	0.0000	0.0000	0.0000	0.0000
52	0.0000	0.0000	0.0000	0.0000

J	QR	QQ	QP	QP	SR
3	1.7431	3.8093	0.5447	0.4305	2.6321
5	2.0310	5.5799	0.9764	0.8223	2.5696
7	1.9809	6.0300	1.1598	1.0075	2.3519
9	1.6969	5.4759	1.1127	0.9832	1.9531
11	1.2984	4.3512	0.9165	0.8178	1.4692
13	0.8956	3.0816	0.6658	0.5974	1.0034
15	0.5600	1.9649	0.4326	0.3893	0.6238
17	0.3186	1.1349	0.2535	0.2284	0.3538
19	0.1654	0.5962	0.1347	0.1214	0.1835
21	0.0785	0.2857	0.0652	0.0586	0.0871
23	0.0341	0.1252	0.0288	0.0258	0.0379
25	0.0136	0.0502	0.0116	0.0104	0.0151
27	0.0050	0.0185	0.0043	0.0038	0.0055
29	0.0017	0.0062	0.0015	0.0013	0.0019
31	0.0005	0.0019	0.0005	0.0004	0.0006
33	0.0001	0.0006	0.0001	0.0001	0.0002
35	0.0000	0.0001	0.0000	0.0000	0.0000
37	0.0000	0.0000	0.0000	0.0000	0.0000
39	0.0000	0.0000	0.0000	0.0000	0.0000
41	0.0000	0.0000	0.0000	0.0000	0.0000
43	0.0000	0.0000	0.0000	0.0000	0.0000
45	0.0000	0.0000	0.0000	0.0000	0.0000
47	0.0000	0.0000	0.0000	0.0000	0.0000
49	0.0000	0.0000	0.0000	0.0000	0.0000
51	0.0000	0.0000	0.0000	0.0000	0.0000

0,0 BAND TEMP 250°K

J	RR	RQ	PP	PQ
2	8.1753	2.7270	0.9034	1.8082
4	9.1350	5.4850	2.8945	4.3451
6	9.5193	6.8046	4.3094	5.7501
8	9.0012	7.0063	4.8867	6.1129
10	7.7616	6.3553	4.7016	5.6461
12	6.1403	5.1997	4.0000	4.6700
14	4.4774	3.8835	3.0701	3.5112
16	3.0194	2.6663	2.1499	2.4203
18	1.8879	1.6906	1.3832	1.5380
20	1.0967	0.9930	0.8214	0.9042
22	0.5927	0.5416	0.4517	0.4931
24	0.2984	0.2747	0.2306	0.2500
26	0.1401	0.1298	0.1095	0.1180
28	0.0614	0.0572	0.0484	0.0519
30	0.0251	0.0235	0.0199	0.0213
32	0.0096	0.0090	0.0077	0.0082
34	0.0034	0.0032	0.0028	0.0029
36	0.0011	0.0011	0.0009	0.0010
38	0.0004	0.0003	0.0003	0.0003
40	0.0001	0.0001	0.0001	0.0001
42	0.0000	0.0000	0.0000	0.0000
44	0.0000	0.0000	0.0000	0.0000
46	0.0000	0.0000	0.0000	0.0000
48	0.0000	0.0000	0.0000	0.0000
50	0.0000	0.0000	0.0000	0.0000
52	0.0000	0.0000	0.0000	0.0000

J	QR	QQ	QP	OP	SR
3	3.4549	7.5515	1.0796	0.8552	5.2103
5	4.1755	11.4739	2.0074	1.6963	5.2708
7	4.2938	13.0729	2.5140	2.1933	5.0811
9	3.9414	12.7213	2.5845	2.2959	4.5171
11	3.2847	11.0094	2.3186	2.0821	3.6970
13	2.5080	8.6310	1.8644	1.6854	2.7921
15	1.7643	6.1914	1.3628	1.2368	1.9511
17	1.1478	4.0889	0.9132	0.8306	1.2642
19	0.6924	2.4962	0.5640	0.5134	0.7609
21	0.3881	1.4127	0.3222	0.2933	0.4261
23	0.2024	0.7428	0.1708	0.1553	0.2222
25	0.0984	0.3634	0.0841	0.0764	0.1081
27	0.0446	0.1656	0.0385	0.0349	0.0490
29	0.0189	0.0704	0.0165	0.0149	0.0208
31	0.0075	0.0279	0.0066	0.0059	0.0082
33	0.0028	0.0104	0.0024	0.0022	0.0030
35	0.0010	0.0036	0.0008	0.0008	0.0011
37	0.0003	0.0012	0.0003	0.0002	0.0003
39	0.0001	0.0004	0.0001	0.0001	0.0001
41	0.0000	0.0001	0.0000	0.0000	0.0000
43	0.0000	0.0000	0.0000	0.0000	0.0000
45	0.0000	0.0000	0.0000	0.0000	0.0000
47	0.0000	0.0000	0.0000	0.0000	0.0000
49	0.0000	0.0000	0.0000	0.0000	0.0000
51	0.0000	0.0000	0.0000	0.0000	0.0000

0,1 BAND TEMP 250°K

J	RR	RQ	PP	PQ
2	4.2282	1.4107	0.4666	0.9342
4	4.7273	2.8390	1.4945	2.2439
6	4.9293	3.5242	2.2241	2.9683
8	4.6641	3.6311	2.5212	3.1544
10	4.0247	3.2961	2.4250	2.9127
12	3.1864	2.6988	2.0626	2.4085
14	2.3253	2.0173	1.5828	1.8105
16	1.5694	1.3862	1.1082	1.2478
18	0.9822	0.8797	0.7129	0.7928
20	0.5711	0.5172	0.4233	0.4661
22	0.3089	0.2824	0.2328	0.2542
24	0.1557	0.1434	0.1188	0.1289
26	0.0732	0.0678	0.0564	0.0608
28	0.0321	0.0299	0.0249	0.0267
30	0.0131	0.0123	0.0103	0.0110
32	0.0050	0.0047	0.0040	0.0042
34	0.0018	0.0017	0.0014	0.0015
36	0.0006	0.0006	0.0005	0.0005
38	0.0002	0.0002	0.0001	0.0002
40	0.0001	0.0001	0.0000	0.0000
42	0.0000	0.0000	0.0000	0.0000
44	0.0000	0.0000	0.0000	0.0000
46	0.0000	0.0000	0.0000	0.0000
48	0.0000	0.0000	0.0000	0.0000
50	0.0000	0.0000	0.0000	0.0000
52	0.0000	0.0000	0.0000	0.0000

J	QR	QQ	QP	OP	SR
3	1.7863	3.9037	0.5582	0.4412	2.6973
5	2.1591	5.9320	1.0380	0.8742	2.7317
7	2.2206	6.7596	1.3002	1.1294	2.6364
9	2.0387	6.5791	1.3369	1.1812	2.3466
11	1.6995	5.6951	1.1996	1.0704	1.9229
13	1.2980	4.4660	0.9649	0.8658	1.4541
15	0.9134	3.2047	0.7056	0.6349	1.0174
17	0.5944	2.1172	0.4730	0.4261	0.6601
19	0.3588	1.2931	0.2922	0.2632	0.3979
21	0.2012	0.7322	0.1670	0.1503	0.2231
23	0.1050	0.3851	0.0886	0.0795	0.1165
25	0.0510	0.1885	0.0436	0.0391	0.0568
27	0.0231	0.0860	0.0200	0.0179	0.0258
29	0.0098	0.0366	0.0086	0.0076	0.0109
31	0.0039	0.0145	0.0034	0.0030	0.0043
33	0.0014	0.0054	0.0013	0.0011	0.0016
35	0.0005	0.0019	0.0004	0.0004	0.0006
37	0.0002	0.0006	0.0001	0.0001	0.0002
39	0.0000	0.0002	0.0000	0.0000	0.0001
41	0.0000	0.0001	0.0000	0.0000	0.0000
43	0.0000	0.0000	0.0000	0.0000	0.0000
45	0.0000	0.0000	0.0000	0.0000	0.0000
47	0.0000	0.0000	0.0000	0.0000	0.0000
49	0.0000	0.0000	0.0000	0.0000	0.0000
51	0.0000	0.0000	0.0000	0.0000	0.0000

0,0 BAND TEMP 300°K

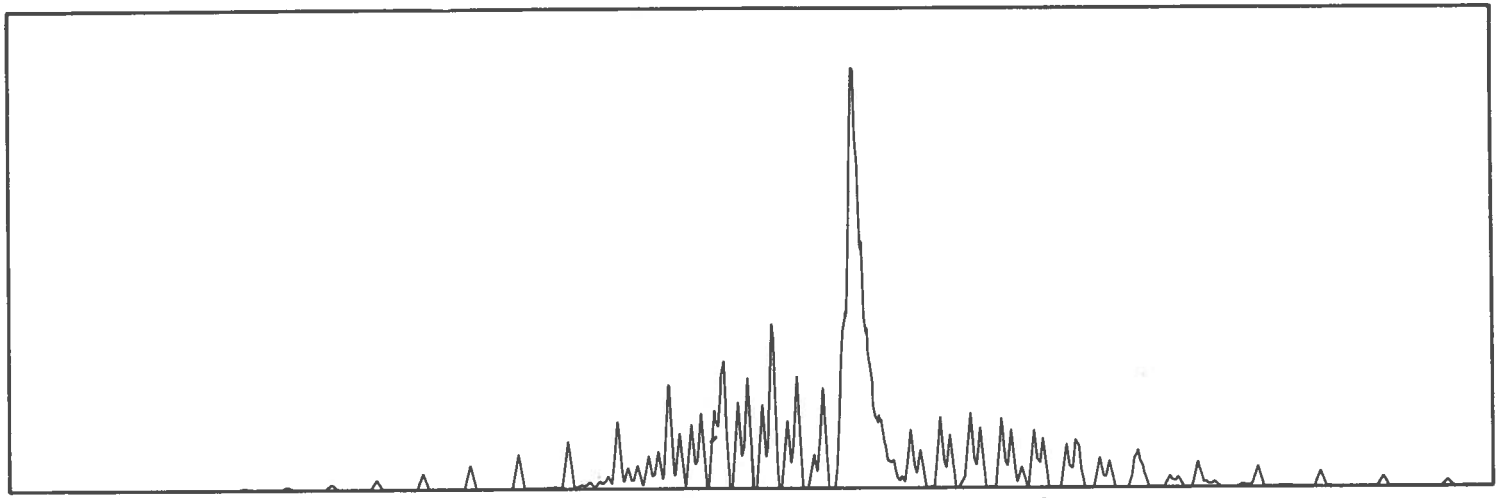
J	RR	RQ	PP	PQ
2	8.2423	2.7494	C.9108	1.8231
4	9.3868	5.6363	2.9743	4.4649
6	10.0788	7.2046	4.5626	6.0881
8	9.9269	7.7269	5.3893	6.7416
10	9.0136	7.3805	5.4600	6.5569
12	7.5907	6.4279	4.9448	5.7731
14	5.9562	5.1661	4.0841	4.6709
16	4.3694	3.8585	3.1111	3.5025
18	3.0044	2.6903	2.2011	2.4474
20	1.9399	1.7566	1.4531	1.5995
22	1.1781	1.0765	0.8979	0.9802
24	C.6737	0.6203	0.5206	C.5644
26	0.3631	0.3365	C.2837	0.3057
28	C.1846	0.1720	C.1455	0.1560
30	C.0886	0.0829	C.0703	0.0751
32	C.0402	0.0378	0.0321	0.0341
34	0.0172	0.0162	0.0138	0.0146
36	C.007C	0.0066	0.0056	0.0059
38	0.0027	0.0025	0.0022	0.0023
40	0.001C	0.0009	C.0008	0.0008
42	0.0003	0.0003	0.0003	C.0003
44	0.0001	0.0001	0.0001	0.0001
46	C.0000	0.0000	0.0000	0.0000
48	0.0000	0.0000	0.0000	0.0000
50	0.0000	0.0000	0.0000	0.0000
52	0.0000	0.0000	0.0000	0.0000

J	QR	QQ	QP	OP	SR
3	3.5117	7.6758	1.0974	0.8693	5.2960
5	4.3494	11.9516	2.0910	1.7669	5.4903
7	4.6335	14.1072	2.7129	2.3668	5.4831
9	4.4544	14.3771	2.9209	2.5947	5.1051
11	3.9303	13.1733	2.7743	2.4914	4.4236
13	3.2119	11.0533	2.3876	2.1584	3.5757
15	2.4447	8.5788	1.8883	1.7138	2.7034
17	1.7395	6.1966	1.3840	1.2587	1.9158
19	1.1602	4.1825	C.9450	0.8602	1.2750
21	0.7268	2.6455	0.6034	0.5492	0.7979
23	C.4282	1.5714	0.3612	0.3285	0.4701
25	0.2376	0.8779	0.2032	0.1845	0.2611
27	0.1243	0.4619	C.1075	0.0975	0.1367
29	0.0613	0.2291	0.0536	0.0485	0.0676
31	C.0286	0.1072	0.0252	0.0227	0.0316
33	0.0126	0.0474	0.0112	0.0101	0.0139
35	0.0052	0.0198	0.0047	0.0042	0.0058
37	0.0021	0.0078	0.0019	0.0017	0.0023
39	C.0008	0.0029	C.0007	0.0006	0.0009
41	0.0003	0.0010	0.0002	0.0002	0.0003
43	0.0001	0.0003	0.0001	0.0001	0.0001
45	0.0000	0.0001	0.0000	0.0000	0.0000
47	0.0000	0.0000	0.0000	0.0000	0.0000
49	0.0000	0.0000	0.0000	0.0000	C.0000
51	0.0000	0.0000	0.0000	0.0000	0.0000

0,1 BAND TEMP 300°K

J	RR	RQ	PP	PQ
2	4.2628	1.4222	C.4705	0.9419
4	4.8576	2.9173	1.5357	2.3057
6	5.2190	3.7314	2.3548	3.1427
8	5.1438	4.0046	2.7805	3.4789
10	4.6739	3.8278	2.8162	3.3825
12	3.9391	3.3363	2.5498	2.9775
14	3.0934	2.6836	2.1055	2.4085
16	2.2712	2.0060	1.6037	1.8057
18	1.5630	1.3999	1.1345	1.2616
20	1.0102	0.9149	C.7489	0.8245
22	0.6141	0.5612	0.4627	0.5052
24	0.3515	0.3237	C.2683	C.2909
26	C.1896	0.1758	0.1462	0.1576
28	C.0965	0.0900	0.0750	0.0804
30	0.0464	0.0434	0.0363	0.0387
32	0.0210	0.0198	0.0165	0.0176
34	0.0090	0.0085	C.0071	0.0075
36	0.0037	0.0035	C.0029	0.0031
38	0.0014	0.0013	0.0011	0.0012
40	0.0005	0.0005	0.0004	0.0004
42	C.0002	0.0002	0.0001	0.0001
44	0.0001	0.0001	C.0000	0.0000
46	0.0000	0.0000	0.0000	0.0000
48	0.0000	0.0000	0.0000	0.0000
50	0.0000	0.0000	0.0000	0.0000
52	0.0000	0.0000	0.0000	0.0000

J	QR	QQ	QP	OP	SR
3	1.8157	3.9679	0.5674	0.4484	2.7417
5	2.2490	6.1789	1.0813	0.9106	2.8455
7	2.3963	7.2945	1.4030	1.2187	2.8450
9	2.3041	7.4354	1.5109	1.3350	2.6521
11	2.0335	6.8144	1.4354	1.2808	2.3009
13	1.6622	5.7194	1.2357	1.1087	1.8622
15	1.2656	4.4404	C.9776	0.8797	1.4098
17	0.9009	3.2086	0.7168	0.6457	1.0004
19	C.6011	2.1666	C.4896	0.4410	0.6667
21	0.3767	1.3710	0.3128	0.2814	0.4178
23	C.2221	0.8148	0.1873	0.1682	0.2465
25	C.1233	0.4554	C.1054	0.0944	0.1371
27	0.0645	0.2398	C.0558	0.0499	0.0719
29	0.0319	0.1190	0.0278	0.0248	0.0356
31	0.0149	0.0557	0.0131	0.0116	0.0167
33	0.0065	0.0246	0.0058	0.0051	0.0074
35	C.0027	0.0103	0.0024	0.0021	0.0031
37	0.0011	0.0041	0.0010	0.0008	0.0012
39	0.0004	0.0015	0.0004	0.0003	0.0005
41	0.0001	0.0005	C.0001	0.0001	0.0002
43	0.0000	0.0002	0.0000	0.0000	0.0001
45	C.0000	0.0001	0.0000	0.0000	0.0000
47	0.0000	0.0000	0.0000	0.0000	0.0000
49	0.0000	0.0000	0.0000	0.0000	0.0000
51	0.0000	0.0000	C.0000	0.0000	0.0000



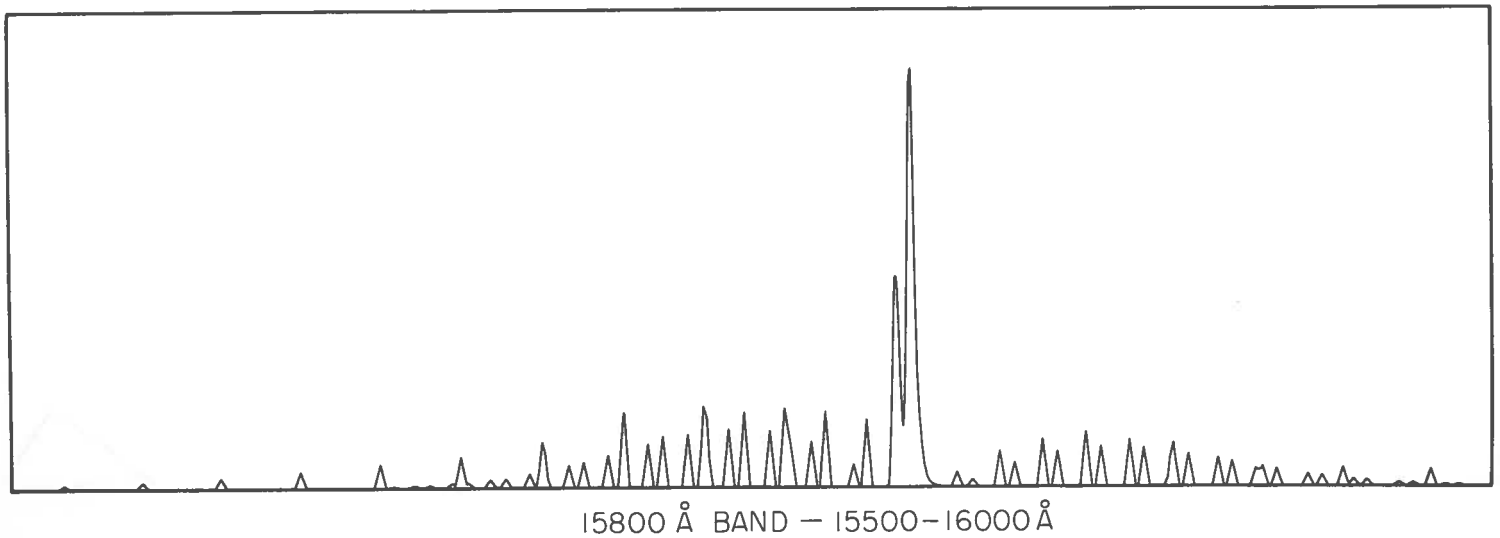


Fig. 2 Theoretical spectrum of the 0,0 and 0,1 bands at 250°K after convolution with a triangular function with a full width of 2Å at half-height.

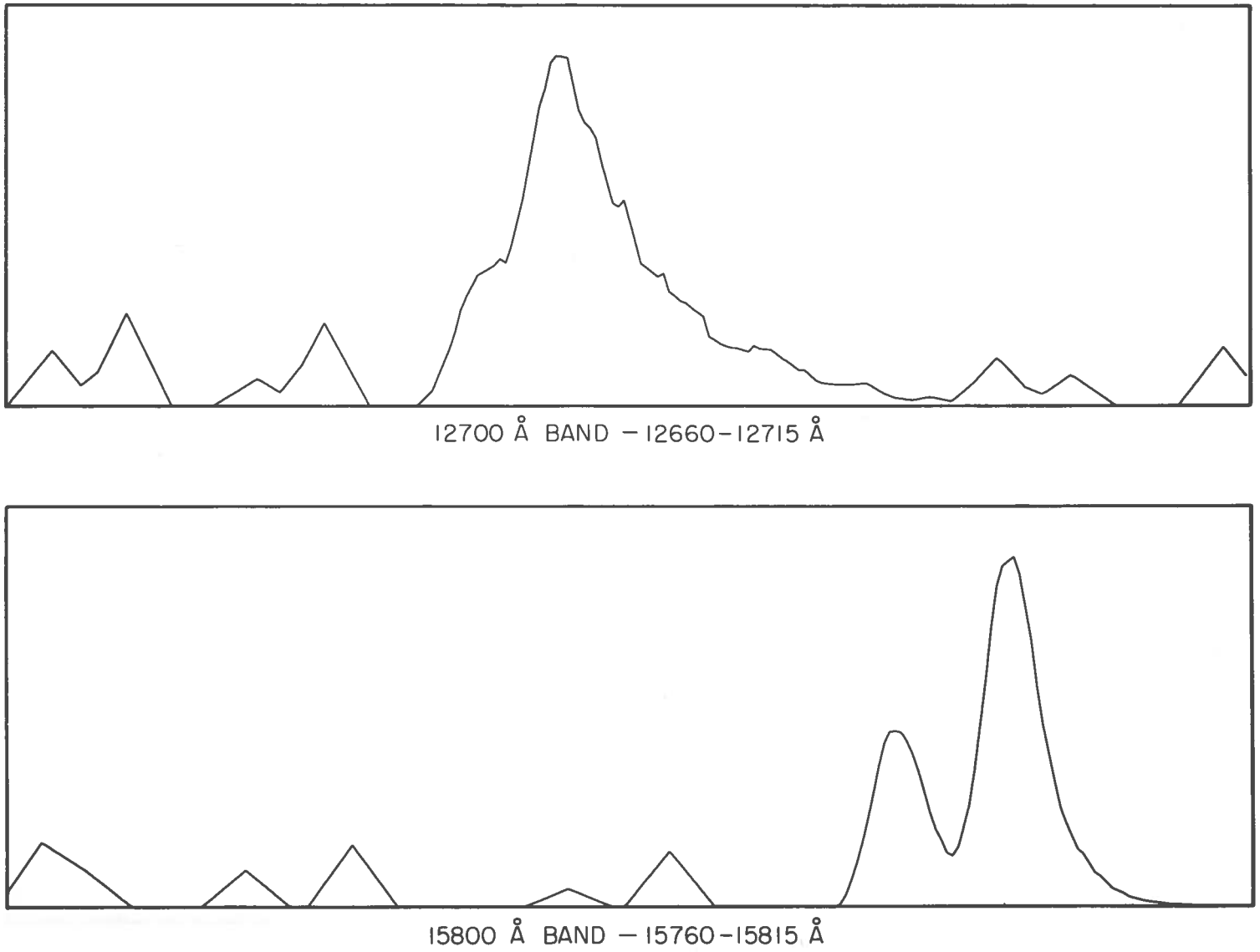


Fig. 3 Theoretical spectrum of the central portion of the 0,0 and 0,1 bands at 250°K after convolution with a triangular function with a full width of 2Å at half-height.

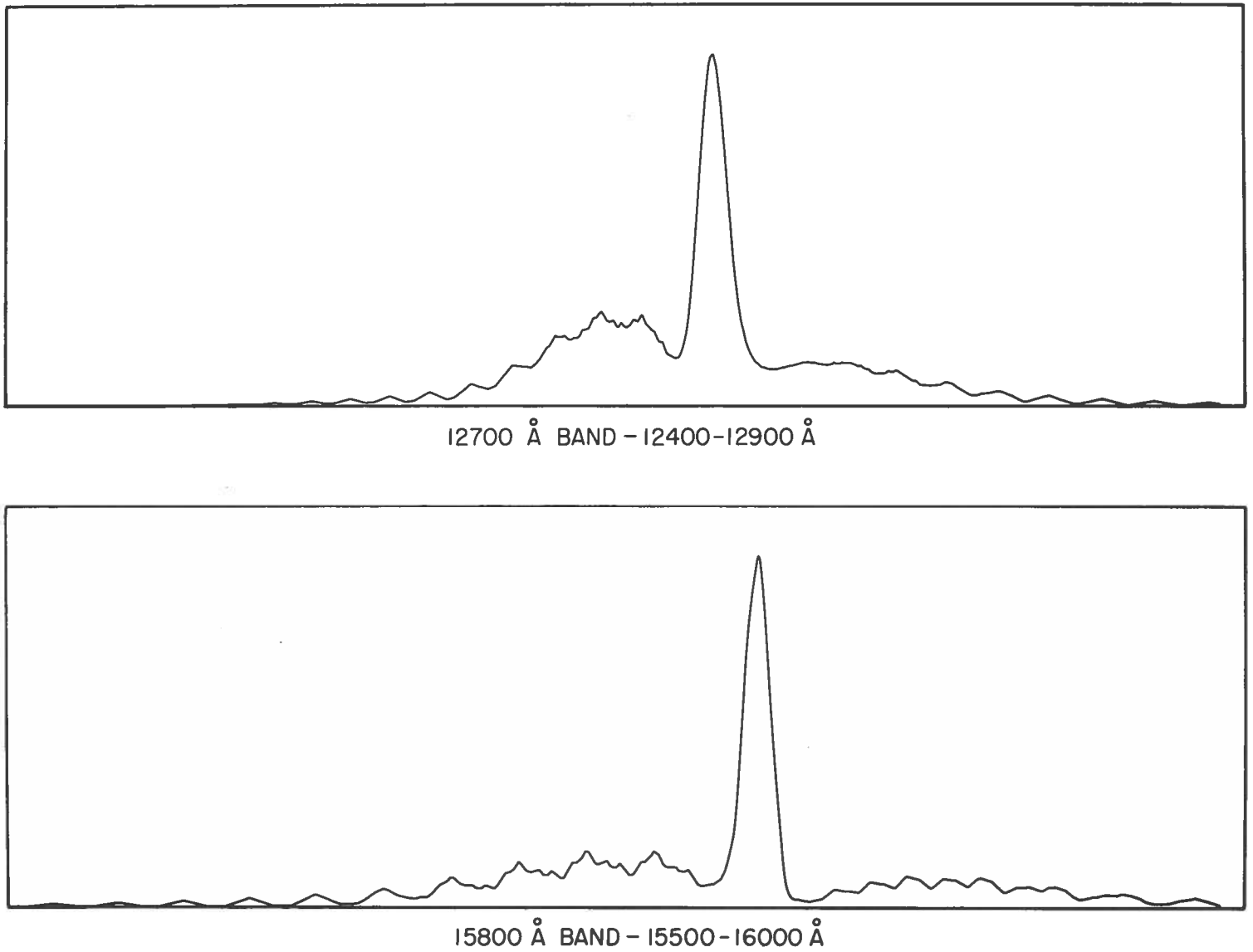
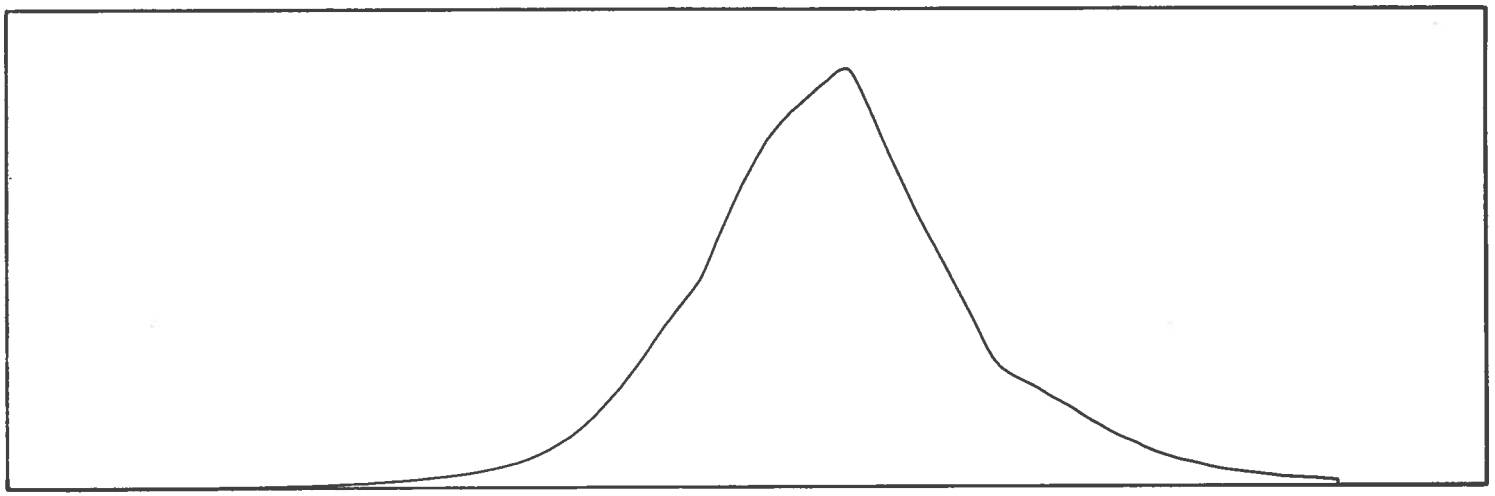
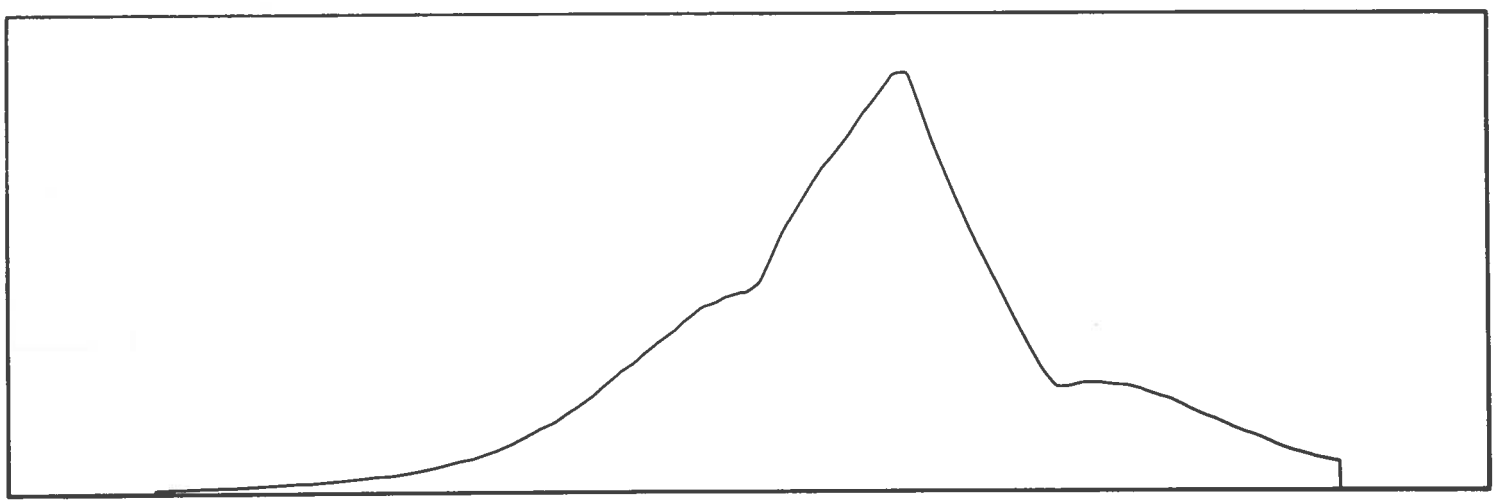


Fig. 4 Theoretical spectrum of the 0,0 and 0,1 bands at 300°K after convolution with a triangular function with a full width of 10Å at half-height.



12700 Å BAND — 12400-12900 Å



15800 Å BAND — 15500-16000 Å

Fig. 5 Theoretical spectrum of the 0,0 and 0,1 bands at 200°K after convolution with a triangular function with a full width of 50Å at half-height.

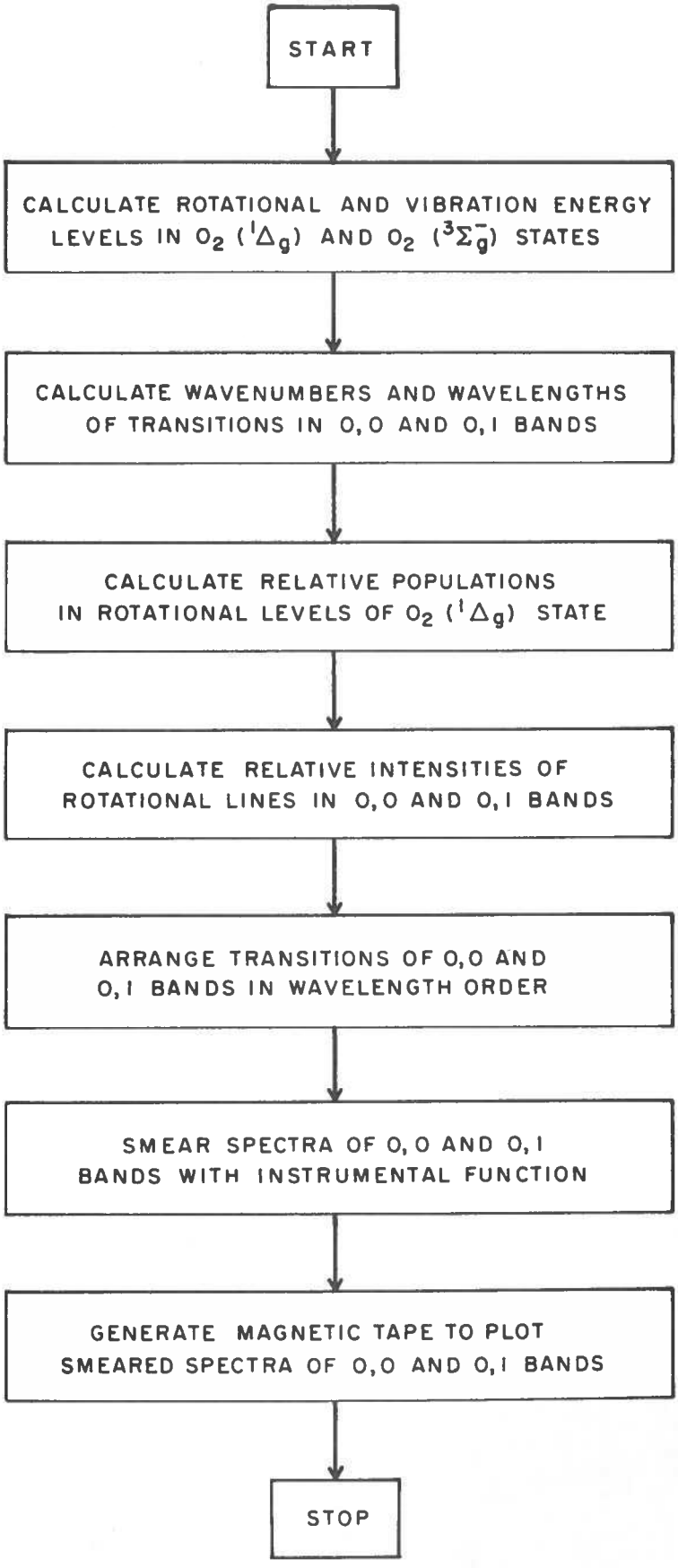


Fig. 6 Flow chart of the computer program written to solve the equations describing the band structure in the $O_2(^1\Delta_g - ^3\Sigma_g^-)$system