Atlas of the Schumann–Runge Absorption Bands of O_2 in the Wavelength Region 175–205 nm

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After a critical summary of previous wavelength measurements and rotational line assignments of the Schumann–Runge absorption bands of O_2, the results of the present study performed at high resolution with a 6.65 m vacuum spectrograph are given. These include (a) an atlas of the Schumann–Runge absorption bands of O_2 at 300 K showing detailed rotational line assignments in the wavelength region 175–205 nm containing the bands $(v',0)$ with $v' = 0$–21 and $(v',1)$ with $v' = 2$–16; (b) tables of wave numbers measured for rotationally assigned principal branch lines belonging to the bands $(v',0)$ with $v' = 0$–17 and $(v',1)$ with $v' = 2$–17; (c) a table of measured wave numbers of lines in the region near the dissociation limit where many unassigned lines exist; (d) a table of wave numbers calculated for satellite and forbidden lines belonging to the bands (9,0)–(17,0) together with the few values obtained from our measurements; and (e) a table of term values for the upper state $B\,^3\Sigma_u^-$ vibration–rotation levels with $v' = 9$–17 calculated from measurements of the principal branch lines of the (9,0)–(17,0) bands and the known ground state term values.

Key words: high resolution photographic atlas; molecular oxygen; rotational assignments; Schumann–Runge absorption bands; term values; wave number tables.

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1. Introduction

The Schumann–Runge bands of O_2, arising from the transition $B\,^3\Sigma_u^- - X\,^3\Sigma_g^-$ between bound states with significantly different equilibrium internuclear distances, are observed in different wavelength regions in absorption (175–205 nm) and emission (211–566 nm). The number of publications on spectroscopic aspects of the Schumann–Runge band system is large, and reviews have been given by Krupenie,[1] Creek and Nicholls,[2] and Huber and Herzberg.[3] In addition, the geophysical fact that solar radiation in the spectral range 175–205 nm of the Schumann–Runge absorption bands plays a crucial role in the photochemistry of the Earth's upper atmosphere is widely recognized, as is the need for accurate measurements of the absorption wavelengths and cross sections of these rotationally discrete bands.[4–6]

In this paper, after a brief description of the Schumann–Runge bands of O_2 (Sec. 2) and a summary of previous measurements (Sec. 3.1), we present in Sec. 3.2 (a) a short account of the experimental procedure (Sec. 3.2.1); (b) an atlas of the Schumann–Runge absorption bands of O_2 at 300 K photographed at high resolution and showing detailed rotational line assignments in the wavelength region 175–205 nm containing the bands $(v',0)$ with $v' = 0$–21 and $(v',1)$ with $v' = 2$–16 (Sec. 3.2.2); (c) tables of wave numbers measured for rotationally assigned principal branch lines belonging to the bands $(v',0)$ with $v' = 0$–17 and $(v',1)$ with $v' = 2$–17 (Sec. 3.2.3); (d) a table of measured wave numbers of lines in the region near the dissociation limit where many unassigned lines exist (Sec. 3.2.4); (e) a table of wave numbers calculated for satellite and forbidden lines belonging to the bands (9,0)–(17,0) together with the few values obtained from our measurements (Sec. 3.2.5); and (f) a table of term values for the upper state $B\,^3\Sigma_u^-$ vibration–rotation levels with $v' = 9$–17 calculated from measurements of the principal branch lines of the (9,0)–(17,0) bands and the known ground state term values (Sec. 3.2.6).

List of Symbols in Tables

B	blended
D	diffuse
W	weak
C	calculated
R	overlapped with a R branch line
P	overlapped with a P branch line
sh	shoulder
?	questionable

2. Brief Description of the Schumann–Runge Absorption Bands of O_2

The Schumann–Runge absorption bands contain many closely spaced rotational lines belonging to 14 branches of this triplet–triplet transition. Most of the observed absorption occurs in the six principal branches, although in the bandhead regions weak satellite and forbidden branches are also seen. In terms of rotational quantum numbers J (representing total angular momentum) and N (representing total angular momentum exclusive of spin), the fine structure levels have, if $N \geqslant 1$, $J = N+1, N, N-1$ and are designated F_1, F_2, F_3, respectively. The selection rules for Hund–Mulliken case b coupling for this $^3\Sigma_u^- - ^3\Sigma_g^-$ transition are $\Delta N = \Delta J = \pm 1$ for the six principal branches R_1, R_2, R_3, P_1, P_2, P_3; $\Delta N = \pm 1$, $\Delta J = 0, \pm 1$, $\Delta N \neq \Delta J$ for the six satellite branches $^RQ_{21}$, $^RQ_{32}$, $^RP_{31}$, $^PQ_{12}$, $^PQ_{23}$, $^PR_{13}$. The branches $^TR_{31}$ and $^NP_{13}$ with $\Delta N = \pm 3$, $\Delta J = \pm 1$ are forbidden in case b coupling. The branch line labels above summarize the quantum number changes shown in the symbol $^{\Delta N}\Delta J_{ij}$ and the subscripts i and j represent, respectively, the upper F_i' and lower F_j'' fine structure levels defining the line transition. (For the principal branches, $i = j$ and $\Delta N = \Delta J$ so that a symbol with a single subscript and no superscript suffices.)

Because $^{16}O_2$ is homonuclear with nuclei of zero spin, only the rotational levels with odd N'' exist in the $^3\Sigma_g^-$ ground state. Energy level diagrams for this $^3\Sigma_u^- - ^3\Sigma_g^-$ transition have been given by Brix and Herzberg[7] and by Julienne.[8] Brix and Herzberg[7] have found that, for all of the unperturbed Schumann–Runge absorption bands with $v' \geqslant 12$, the order of increasing wave number of the principal branch lines is P_1, P_2, P_3, and R_1, R_2, R_3. The triplet splitting parameters for the ground state are considered in detail by Veseth and Loftus[9] and by Mizushima[10]; the splitting parameters of the B state and their dependence on v' have been calculated by Bergeman and Wofsy[11] from the experimental data available in 1972.

The Schumann–Runge bands $(v'0)$ vary greatly in intensity, having oscillator strengths[12–16] that increase as v' increases from 0 to 14 and then decrease gradually as v' increases further. Each band has a head at short wavelength and is degraded towards long wavelength. The upper state of the band system is predissociated, with the result that individual rotational linewidths depend quite strongly on v'. The predissociation has been investigated theoretically,[8,17–20] and Julienne[8] has found that a repulsive $^5\Pi_u$ state is primarily though not exclusively responsible for the predissociation. In experimental studies by Gies *et al.*,[13] Lewis *et al.*,[14,15] and Frederick and Hudson[16] predissociation linewidths (FWHM) ranging from 0.1 to 4 cm^{-1} have been found, with maxima occurring for $v' = 4,7,11$. Linewidths of greater accuracy will become available from an analysis, currently in progress,[21] of the absolute cross section data of Yoshino *et al.*[12] Predissociation in the B state is so extensive for $v' > 3$ that emission or fluorescence from levels with $v' > 3$ is seldom observed, and then only feebly under the most energetic excitation conditions.[2,22]

3. Photographic Atlas, Rotational Line Positions, and Assignments of the Schumann–Runge Absorption Bands of O_2

3.1. Previous Measurements

Wavelength measurements and useful photographic reproductions of the Schumann–Runge absorption bands exist in publications by Curry and Herzberg[23] ($v' = 1$–7, $v'' = 0$), Knauss and Ballard[24] ($v' = 8$–15, $v'' = 0$), Brix and Herzberg[7] ($v' \geqslant 12$, $v'' = 0$), Ogawa[25] ($v' = 5$–10, $v'' = 0$–5), Ogawa and Chang[26] ($v' = 5$–18, $v'' = 0$–3), Hudson and Carter[27] ($v' = 6$–17, $v'' = 0$–2), and Biaumé[28] ($v' = 0$–13, $v'' = 0$; $v' = 4$–13, $v'' = 1$). Yoshino *et al.*[12] have presented graphically the absorption cross sections of the bands with $v' = 1$–12, $v'' = 0$, and $v' = 3$–16, $v'' = 1$ from high resolution data stored on magnetic tape; the same instrumentation has been used by Smith *et al.*[29] to measure the oscillator strengths of lines of astrophysical interest belonging to the (13,0)–(16,0) bands. The wavelengths used in those works[12,29] were obtained from the photographic measurements given in the present paper. A photographic atlas of the emission bands with $v' = 0$–5 and $v'' = 6$–21 at moderate resolution in the region 232–442 nm has been prepared by Hébert *et al.*,[30] and Creek and Nicholls[2] have assigned 5400 of the 7700 measured emission lines in the region 211–566 nm to 87 bands of the system, though without consideration of the triplet fine structure.

The most recent wavelength measurements and rotational analyses of the (v',0) absorption bands are those of Brix and Herzberg[7] for $v' \geqslant 12$ and of Ackerman and Biaumé[31] for $v' = 0$–13. The measurements of Ackerman and Biaumé[31] and of Biaumé[28] are essentially identical. These absorption studies[28,31] were performed in the fourth order of a 1200 lines/mm grating in the same 3 m vacuum spectrograph used by Brix and Herzberg.[7] Comparison of the (12,0) and (13,0) bands of these studies reveals several instances in which Brix and Herzberg[7] resolve $P_2(N)$ from $P_3(N)$ or $R_2(N)$ from $R_3(N)$ while Ackerman and Biaumé[31] do not.

3.2. Present Measurements

3.2.1. Experimental Procedure

A 6.65 m scanning spectrometer/spectrograph, described previously,[32] has been used with an entrance slit width of 10 μm to photograph the Schumann–Runge bands of O_2 at a reciprocal dispersion of 0.06 nm/mm in the first order of a 2400 lines/mm grating. This is the same instrument that was used photoelectrically for our recent high resolution cross section measurements[12] and oscillator strength determinations[12,29] of the Schumann–Runge bands. The background continuum is obtained from a condensed discharge in xenon or from a dc discharge in hydrogen. Typical exposure times with Kodak SWR plates are 2–10 min. For wavelength calibration, the fourth positive emission bands of CO are used. Wavelength measurements, performed with a Grant comparator, have a relative accuracy of 0.0001 nm for the sharpest lines, and the absolute accuracy is 0.0003 nm.

The spectra in Figs. 1 and 2 for the (0,0) and (1,0) bands and the upper spectra in Figs. 3–5 for the (2,0), (3,0), and (4,0) bands are obtained from air at pressures up to 760 Torr (0.1 MPa), nominally at 300 K, in the interior of the 6.65 m spectrograph which provides an optical path length of 13.3 m. The lower spectra in Figs. 3–5 for the (2,0), (3,0), and (4,0) bands and all the spectra in Figs. 6–18 for the (5,0) bands through to the dissociation limit are obtained from O_2 at 300 K in a 20 cm cell in front of the entrance slit of the spectrograph.

The wave numbers given in Tables 1–4 have been measured from the plates corresponding to Figs. 1–18 and from other plates of the spectra obtained from air (300 K, 50–760 Torr) or O_2 (300 K, 0.001–0.175 Torr) in the interior of the spectrograph, and from O_2 (300 K, 0.4–1000 Torr; 77 K, 0.1–40 Torr; 615 K, 4–7 Torr) in the external 20 cm long cell. In all cases, the CO lines of known vacuum wavelength used for calibration were photographed in the first order of the 2400 lines/mm grating after passage through the sample of air or O_2 under study.

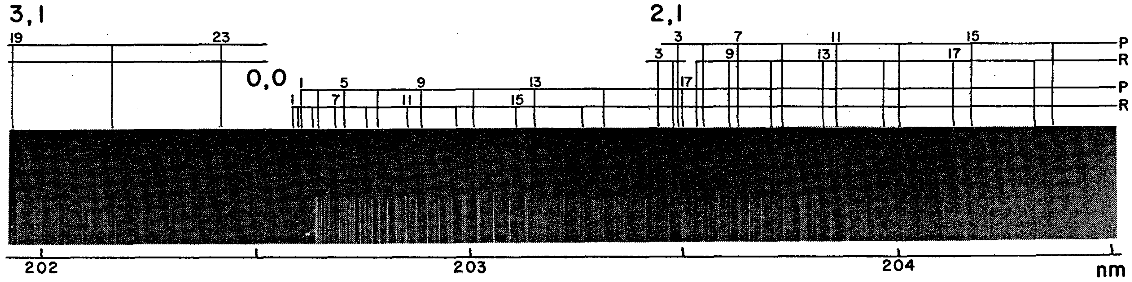

FIG. 1. The (0,0) Schumann–Runge band region of O_2.

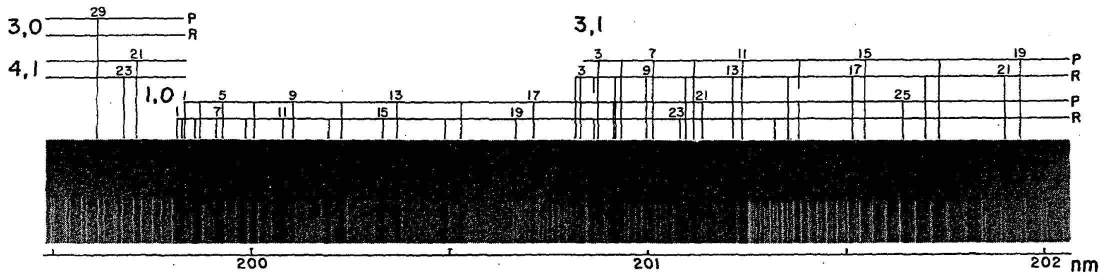

FIG. 2. The (1,0) Schumann–Runge band region of O_2.

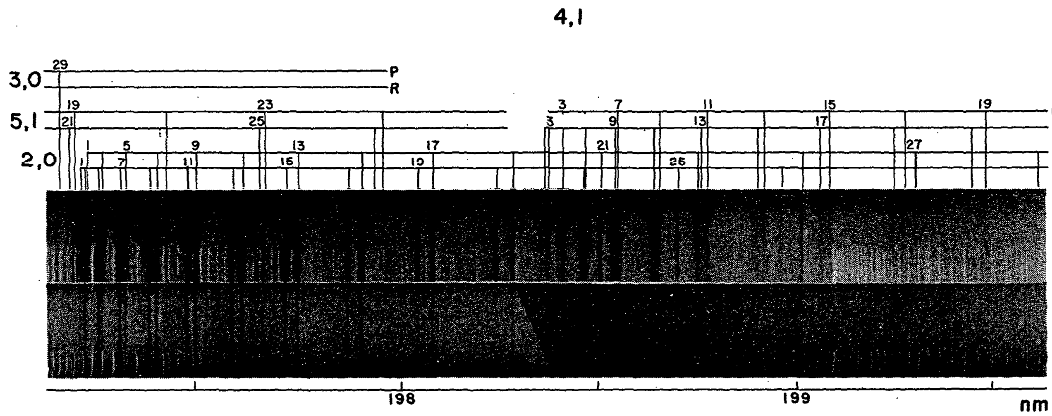

FIG. 3. The (2,0) Schumann–Runge band region of O_2.

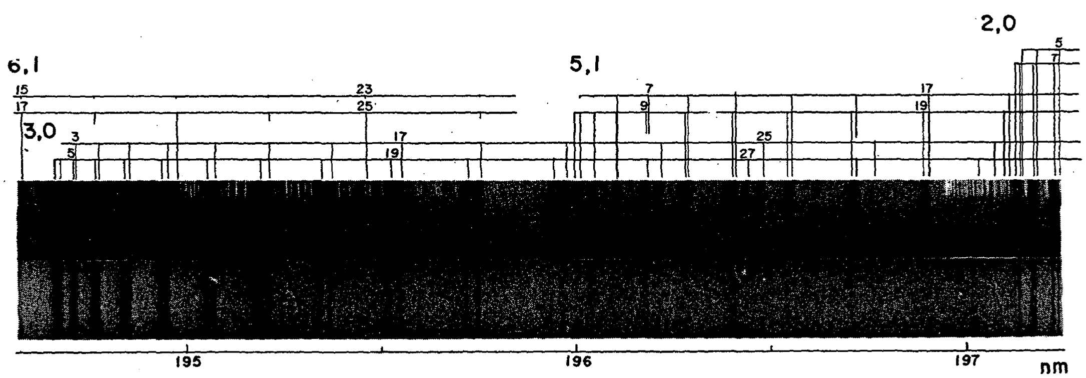

FIG. 4. The (3,0) Schumann–Runge band region of O_2.

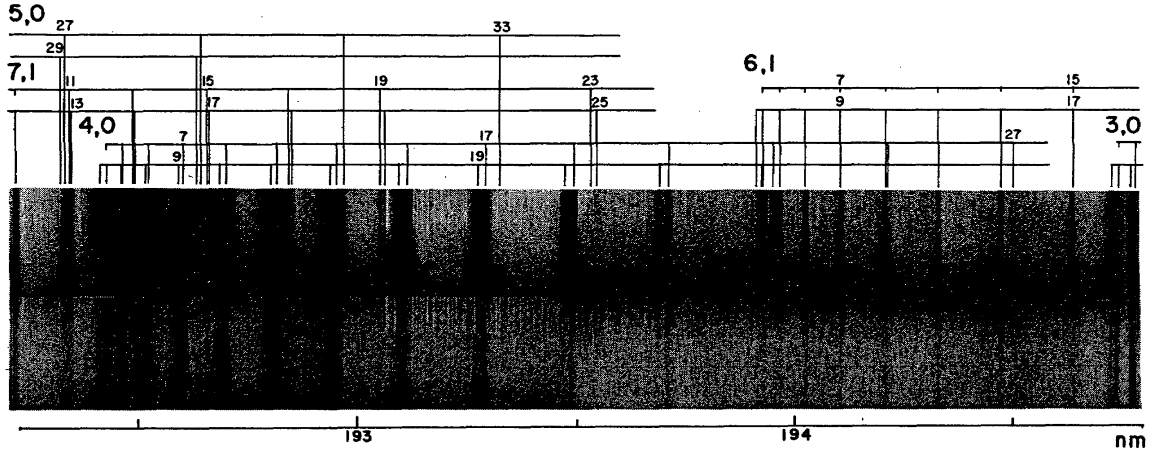

FIG. 5. The (4,0) Schumann–Runge band region of O_2.

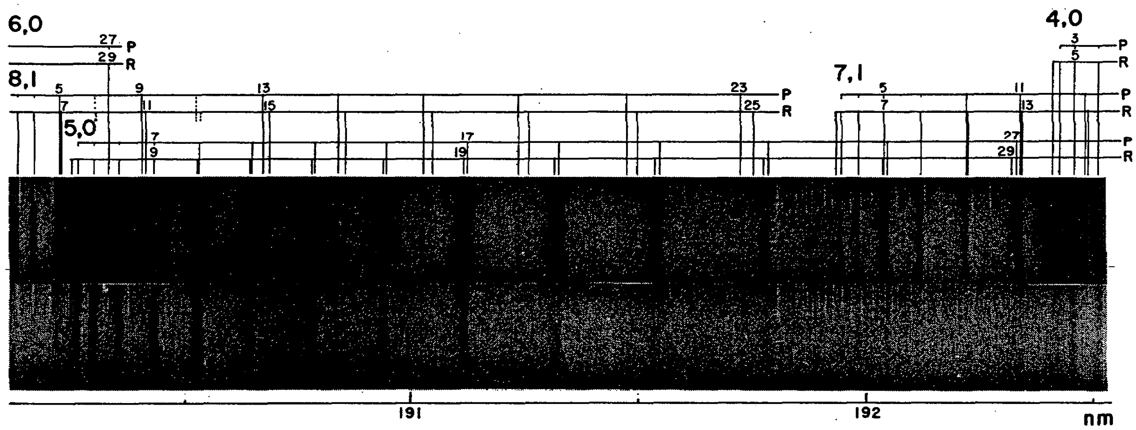

FIG. 6. The (5,0) Schumann–Runge band region of O_2.

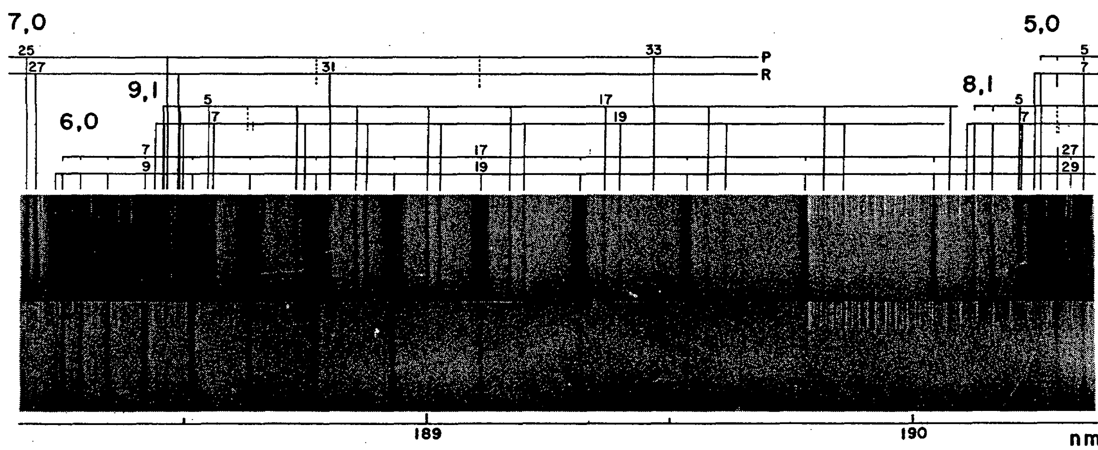

FIG. 7. The (6,0) Schumann–Runge band region of O_2.

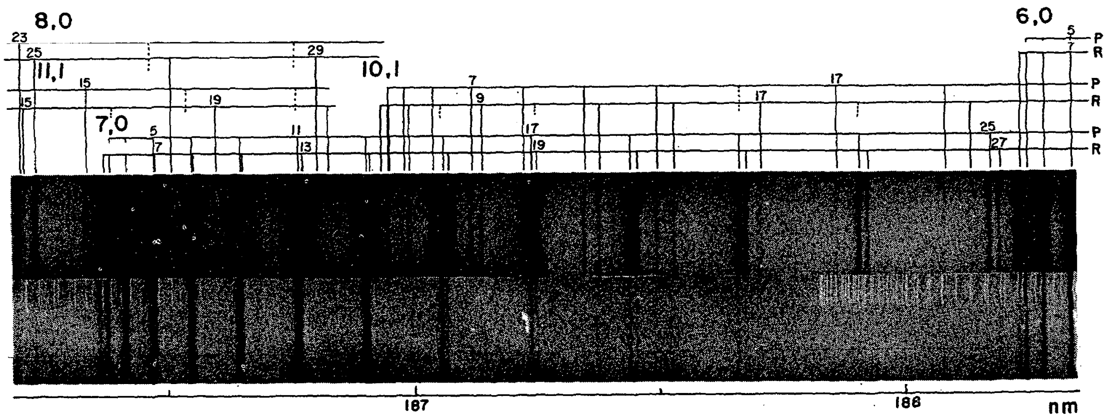

FIG. 8. The (7,0) Schumann–Runge band region of O_2.

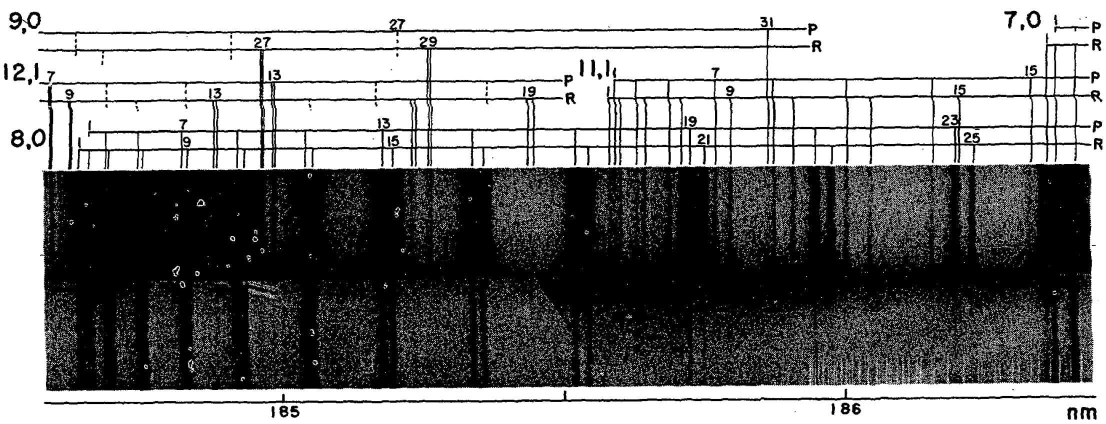

FIG. 9. The (8,0) Schumann–Runge band region of O_2.

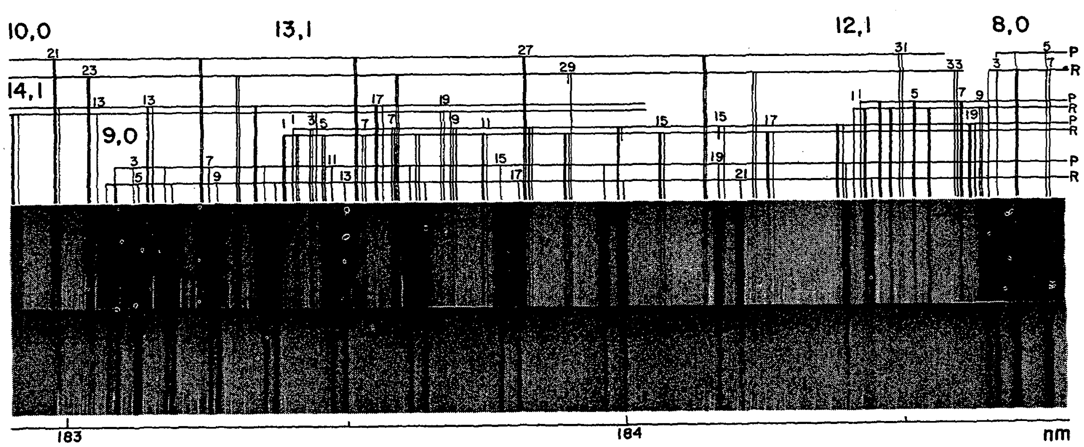

FIG. 10. The (9,0) Schumann–Runge band region of O_2.

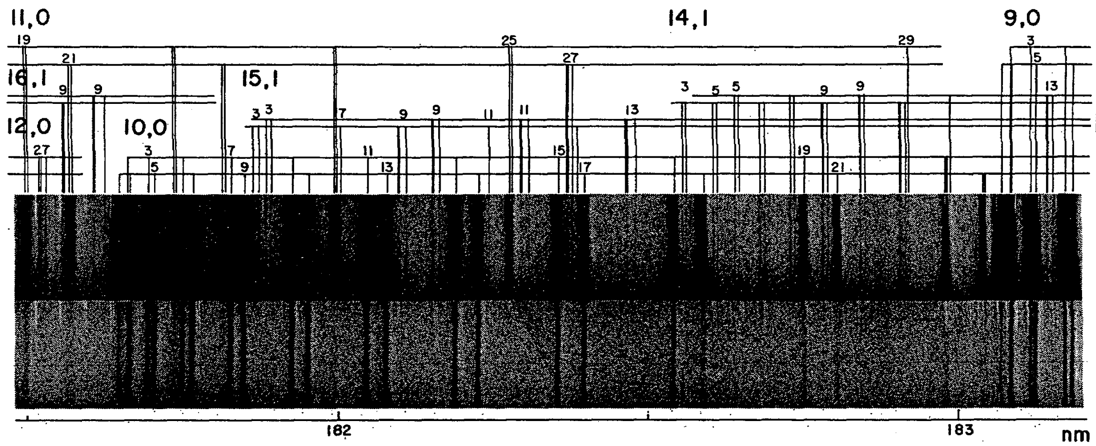

FIG. 11. The (10,0) Schumann–Runge band region of O_2.

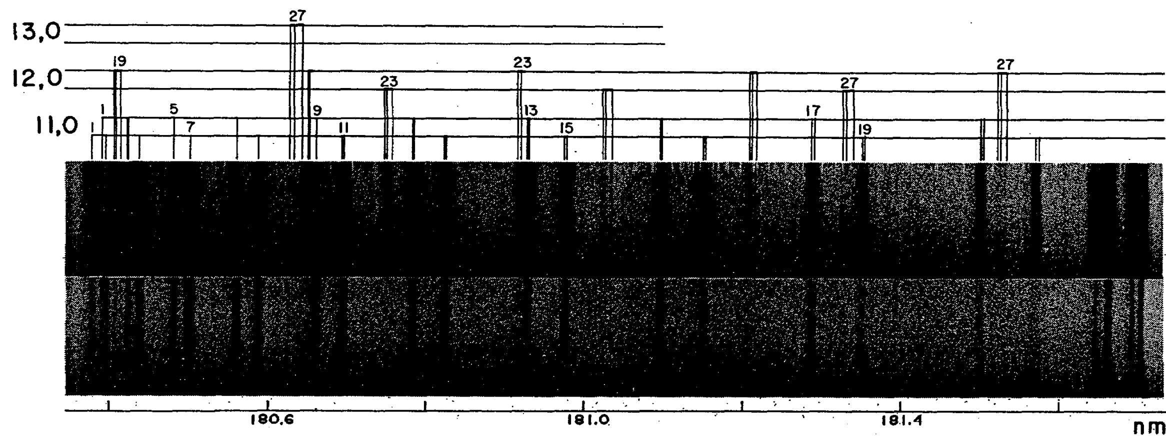

FIG. 12. The (11,0) Schumann–Runge band region of O_2.

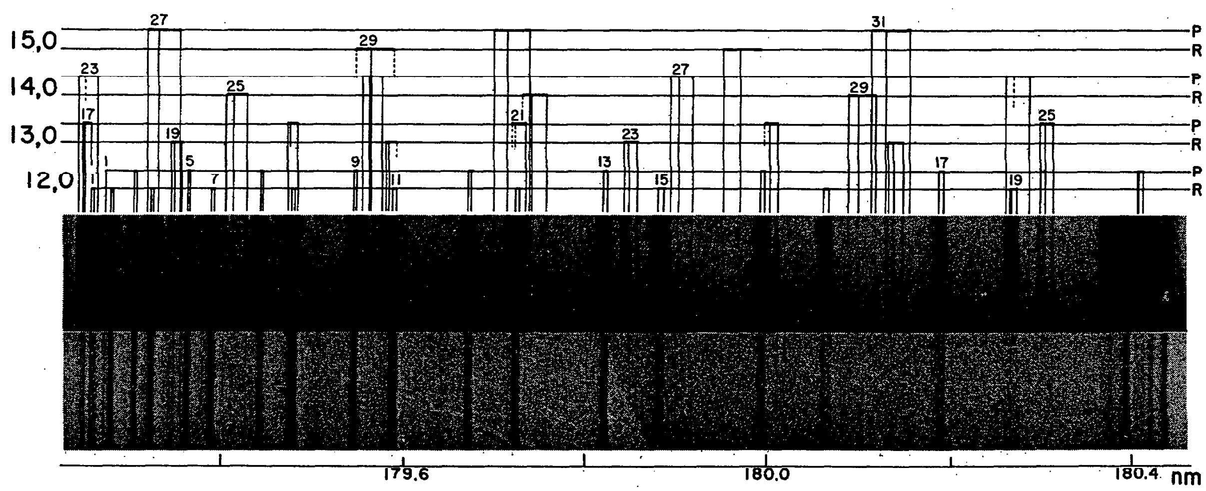

FIG. 13. The (12,0) Schumann–Runge band region of O_2.

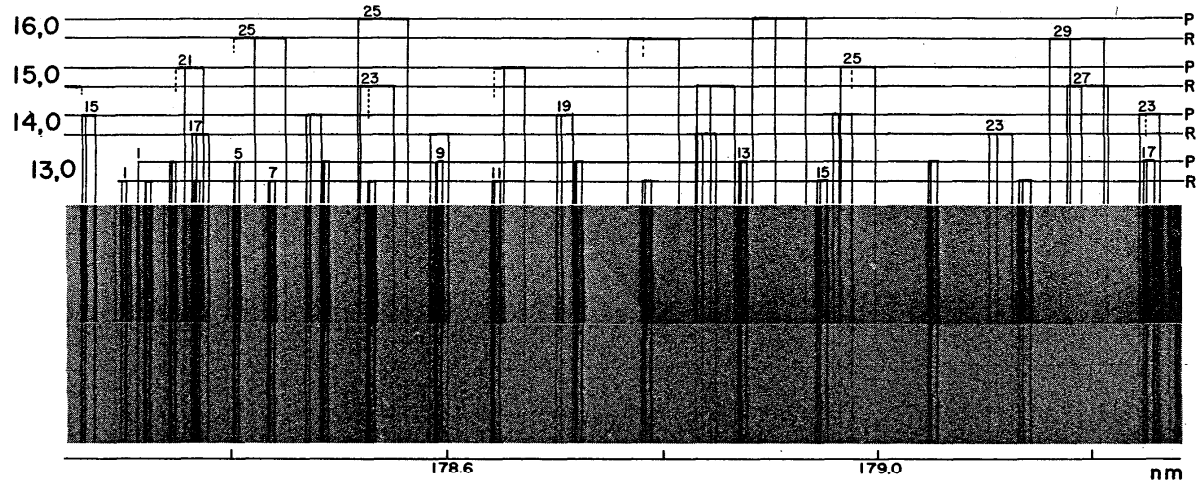

FIG. 14. The (13,0) Schumann–Runge band region of O_2.

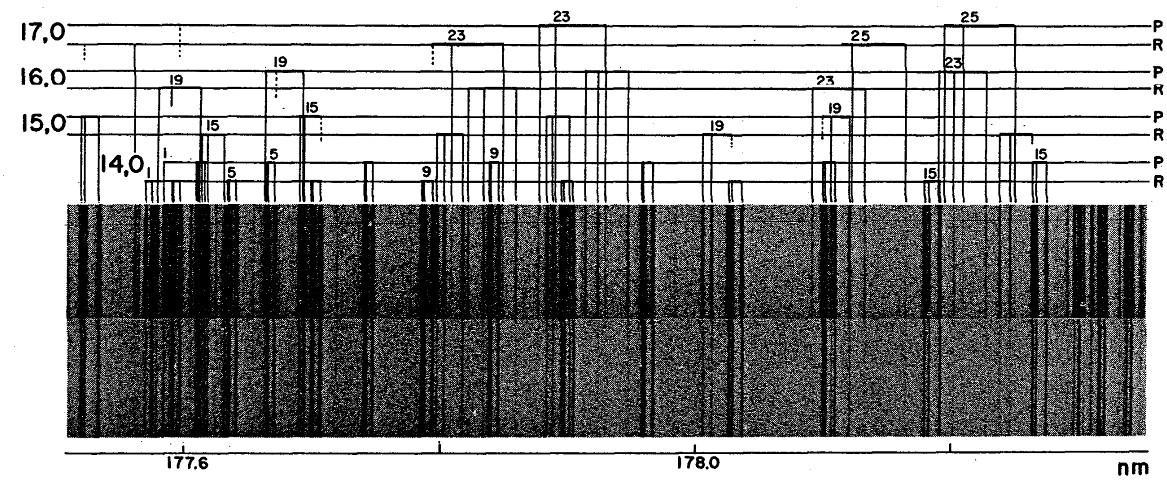

FIG. 15. The (14,0) Schumann–Runge band region of O_2.

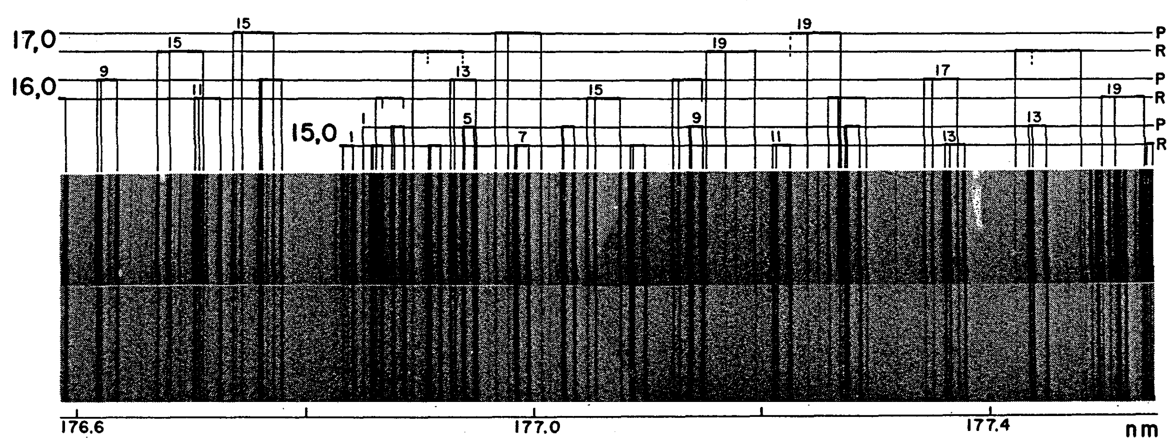

FIG. 16. The (15,0) Schumann–Runge band region of O_2.

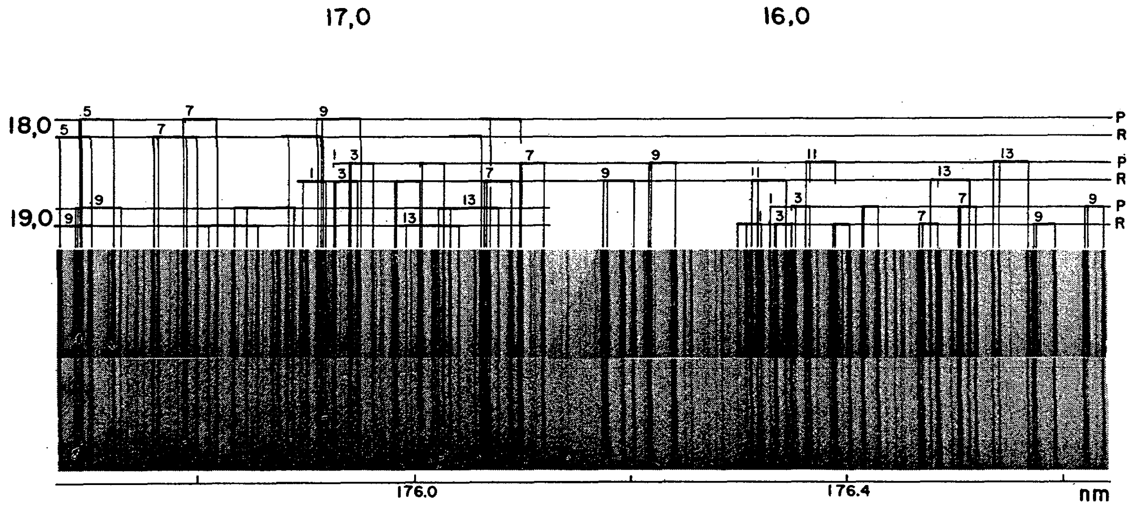

FIG. 17. The (16,0) and (17,0) Schumann–Runge band region of O_2.

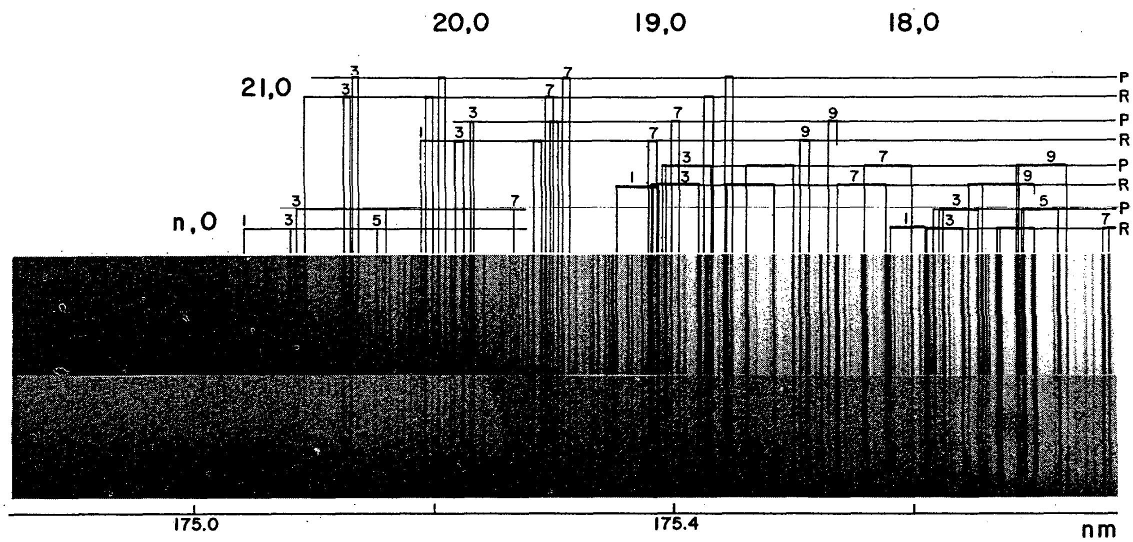

FIG. 18. The (18,0)–(21,0) Schumann–Runge band region of O_2.

Table 1.0. Wave numbers of the B(0)-X(0) band

N	R(N)	P(N)
1	49360.00	
3	49357.11	49345.70
5	49349.01	49331.20
7	49335.97	49311.67
9	49317.96	49287.16
11	49294.97	49257.69
13	49266.97	49223.18
15	49233.89	49183.73

Table 1.1. Wave numbers of the B(1)-X(0) band

N	R(N)	R(N)sh	P(N)	P(N)sh
1	50047.45		50042.80	
3	50044.40		50033.19	
5	50036.05		50018.51	
7	50022.64	50022.93B	49998.70	
9	50004.14	50004.48B	49973.79	49974.08B
11	49980.44	49980.89B	49943.76	49944.15B
13	49951.70	49952.16B	49908.65	49909.18B
15	49917.84	49918.57B	49868.46	49868.97B
17	49878.96	49879.58B	49823.15	49823.77B
19	49834.85	49835.57B	49772.71	
21	49785.55		49717.33	
23	49731.35			

Table 1.2. Wave numbers of the B(2)–X(0) band

N	R(N)	R(N)sh	P(N)	P(N)sh
1	50712.56		50707.92	
3	50709.24	50709.51B	50698.31	
5	50700.61	50701.01B	50683.38	50683.65B
7	50686.80	50687.10B	50663.28	50663.66B
9	50667.75	50668.27B	50637.94	50638.35B
11	50643.46	50644.08B	50607.41	50607.80B
13	50613.95	50614.50B	50571.66	50572.13B
15	50579.23	50579.92B	50530.68	50531.29B
17	50539.27	50540.08B	50484.53	50485.22B
19	50494.06	50494.98B	50433.10	50433.87B
21	50443.61	50444.64B	50376.49	50377.51B
23	50388.01	50388.69B	50314.67	50315.57B
25	50327.10	50327.78B	50247.70	50248.60B
27	50261.09	50261.49B	50175.44	

Table 1.3. Wave numbers of the B(3)–X(0) band

N	R(N)	P(N)
1	51353.65	
3	51350.26	51339.74
5	51341.23	51324.47
7	51327.02	51303.98
9	51307.42	51278.21
11	51282.50	51247.12
13	51252.19	51210.67
15	51216.54	51168.90
17	51175.52	51121.87
19	51129.19	51069.43
21	51077.48	51011.66
23	51020.43	50948.59
25	50957.74	50880.11
27	50890.28	50806.39
29	50818.46	50727.12

Table 1.4. Wave numbers of the B(4)–X(0) band

N	R(N)	P(N)
1	51970.44B	51967.25R
3	51967.25	51956.80B
5	51957.62	51942.09
7	51942.90	51921.07
9	51921.51	51894.70
11	51897.84	51862.85
13	51865.85	51825.67
15	51829.29	51783.07
17	51787.27	51735.01
19	51739.64	51681.42
21	51686.70	51622.47
23	51628.01	51557.89
25	51565.56	51488.34B
27	51494.17	51412.99

Table 1.5. Wave numbers of the B(5)–X(0) band

N	R(N)	P(N)
1	52562.47	52559.67B
3	52558.68	52548.61B
5	52548.88	52533.05B
7	52533.52	52512.11B
9	52512.53	52485.07
11	52486.14	52452.75
13	52454.03	52414.78
15	52416.37	52371.15
17	52373.09	52321.98
19	52324.25	52267.26
21	52269.60	52206.88
23	52209.35	52140.88
25	52143.49	52069.59
27	52070.92[a]	51991.96
29	51994.85	51909.19
31	51912.44	
33		51726.48

[a] Overlapped with a line of (7,1) band.

Table 1.6. Wave numbers of the B(6)–X(0) band

N	R(N)	P(N)
1	53124.02	53119.88R
3	53119.88P	53109.83R
5	53109.83P	53094.01R
7	53094.01P	53072.45R
9	53072.45P	53045.10R
11	53045.10P	53012.03R
13	53012.03P	52973.23R
15	52973.23P	52928.63R
17	52928.63P	52878.34R
19	52878.34P	52822.24R
21	52822.24P	52760.45R
23	52760.45P	52692.84R
25	52692.84P	52619.59R
27	52619.59P	52540.38R
29	52540.38P	

Table 1.7. Wave numbers of the B(7)–X(0) band

N	R(N)	R(N)sh	P(N)	P(N)sh
1	53657.29		53653.07R	
3	53653.07P		53642.80	
5	53642.80		53626.66	
7	53626.11		53604.96	
9	53603.92		53577.03	
11	53575.72		53543.43	
13	53541.51		53503.64	
15	53501.31		53458.07	
17	53455.17		53406.51	53406.89B
19	53403.29	53403.67B	53349.02	53349.37B
21	53345.22	53345.73B	53285.53	53286.21B
23	53281.18	53281.60B	53216.12	53216.57B
25	53211.15	53212.00B	53140.93	53141.56B
27	53135.27	53135.97B	53059.69	
29	53053.01		52972.26C	
31	52965.49		52878.72C	
33			52779.61C	

Table 1.8. Wave numbers of the B(8)-X(0) band

N	R(N)	P(N)
1	54157.41	54153.10B
3	54152.45	54142.76B
5	54141.68	54126.47
7	54124.48	54104.07
9	54101.34	54075.54
11	54072.00	54040.90
13	54036.63	54000.15
15	53995.16	53953.39
17	53947.55	53900.42
19	53893.80	53841.40
21	53833.95	53776.27
23	53767.89	53704.97
25	53695.72	53627.53C
27	53617.50	53544.02C
29	53532.46?	53454.48C
31		53357.75C

Table 1.9. Wave numbers of the B(9)-X(0) band

N	$R_1(N)$	$R_2(N)$	$R_3(N)$	$P_1(N)$	$P_2(N)$	$P_3(N)$
1	54622.92	54625.23B		54618.43B		
3	54617.83			54608.64	54609.34B	
5	54606.33	54606.69B		54592.01	54592.40B	
7	54588.54	54588.99B		54569.00	54569.28B	
9	54564.38	54564.74B		54539.68	54539.91B	
11	54533.95	54534.25B		54504.05	54504.35B	
13	54497.23	54497.68B		54462.15	54462.56B	
15	54454.07	54454.48B		54413.88	54414.40B	
17	54404.62	54405.14B		54359.35	54359.81B	54360.13B
19	54348.66	54349.43B	54349.91B	54298.48	54298.88B	54299.35B
21	54286.83	54287.27B	54287.71B	54231.35	54231.93B	
23	54218.35	54218.84B	54219.45B	54157.70		
25	54143.01			54078.07		
27	54062.12	54063.44B		53992.21		
29	53974.61	53975.63B	53976.76B			
31				53800.14	53801.40B	

Table 1.10. Wave numbers of the B(10)-X(0) band

N	$R_1(N)$	$R_2(N)$	$R_3(N)$	$P_1(N)$	$P_2(N)$	$P_3(N)$
1	55051.53	55053.76		55047.37		
3	55046.20			55037.34		
5	55034.16	55033.81		55020.16	55020.35	
7	55015.37	55015.62		54996.60	54996.80	
9	54990.14	54990.51		54966.35	54966.64	
11	54958.32	54958.79		54929.75	54930.04	
13	54920.11	54920.64		54886.65	54886.99	
15	54875.29	54876.00		54836.87	54837.35	
17	54823.97	54824.71	54825.15	54780.64	54781.33	
19	54765.99	54766.86	54767.08	54717.71	54718.60	54718.98
21	54701.46	54702.52	54703.09	54648.52	54649.26	54649.66
23	54630.27	54631.32	54631.94	54572.50	54573.38	54573.90
25	54552.45	54553.64	54554.20	54489.98	54491.08	54491.67
27	54467.89	54469.08	54469.59	54400.78	54401.96	
29	54376.64	54377.93		54304.94	54306.03	54306.81
31	54278.70	54280.12	54281.15	54202.42	54203.63	
33				54093.09		

Table 1.11. Wave numbers of the B(11)-X(0) band

N	$R_1(N)$	$R_2(N)$	$R_3(N)$	$P_1(N)$	$P_2(N)$	$P_3(N)$
1	55439.23			55435.30B		
3	55433.59			55425.12	55425.60B	
5	55420.89			55407.67	55407.99B	
7	55401.31			55383.61		
9	55374.80B	55375.16		55352.17	55352.54	55352.93
11	55341.54	55342.12		55314.42B	55314.88	
13	55301.77	55302.46		55269.85B	55270.40	
15	55255.02	55255.88		55218.42	55219.08	
17	55201.46	55202.57		55160.19	55160.74	55161.25
19	55140.97	55142.37		55095.37	55096.37	
21	55073.77	55075.11	55075.56	55023.52	55024.66	55025.15
23	54999.39	55001.02		54944.86	54946.14	54946.66
25				54859.91	54860.91	
27	54830.36	54832.12	54833.37			
29				54667.40		

Table 1.12. Wave numbers of the B(12)-X(0) band

N	$R_1(N)$	$R_2(N)$	$R_3(N)$	$P_1(N)$	$P_2(N)$	$P_3(N)$
1	55784.16	55784.94	55787.29	55780.63		
3	55777.76	55778.53	55778.68	55769.91	55770.61	55771.11
5	55764.20	55765.01	55765.16	55751.93	55752.69P	55752.69P
7	55743.59	55744.51	55744.75	55726.87	55727.62	55727.80
9	55715.88	55716.98	55717.18	55694.76	55695.68	55695.87
11	55681.14	55682.45	55682.64	55655.58	55656.55	55656.85
13	55639.42	55640.66	55641.06	55609.37	55610.51	55610.85
15	55590.41	55591.88	55592.34	55556.08	55557.41	55557.95
17	55534.37	55535.94	55536.58	55495.73	55497.16	55497.66
19	55471.18	55472.86	55473.59	55428.23	55429.81	55430.44
21					55355.22	55356.05
23	55323.13	55325.19	55326.28		55273.58	55274.33
25	55238.21	55239.52	55240.36	55182.84	55184.85	55185.77
27	55145.94	55148.35	55149.59	55086.54	55088.76	55090.24

Table 1.13. Wave numbers of the B(13)-X(0) band

N	$R_1(N)$	$R_2(N)$	$R_3(N)$	$P_1(N)$	$P_2(N)$	$P_3(N)$
1	56084.39	56085.68	56088.10	56081.06		
3	56077.40	56078.67	56078.98	56070.13	56071.31	56071.87
5	56062.98	56064.32	56064.54	56051.59	56052.82	56053.01
7	56041.17	56042.63	56042.96	56025.63	56027.08P	56027.08P
9	56011.99	56013.54	56014.04	55992.34	55993.77	55994.06
11	55975.44	55977.14	55977.73	55951.66	55953.21	55953.67
13	55931.46	55933.30	55934.04	55903.63	55905.31	55905.89
15	55880.05	55882.09	55882.97	55848.19	55850.04	55850.75
17	55821.12	55823.35	55824.47	55785.30	55787.38	55788.18
19	55754.68	55757.14	55758.44	55714.97	55717.18	55718.21
21	55681.14B	55683.29B	55684.82	55637.15	55639.42B	55641.06B
23	55599.11	55601.99	55603.67	55551.75	55554.38	55556.08
25	55509.80	55513.02	55514.85	55458.83	55461.69	55463.38
27				55358.26	55361.28	55363.25

Table 1.14. Wave numbers of the B(14)-X(0) band

N	$R_1(N)$	$R_2(N)$	$R_3(N)$	$P_1(N)$	$P_2(N)$	$P_3(N)$
1	56338.61	56340.46	56342.87?	56335.42		
3	56330.99	56332.89	56333.09	56324.28	56326.06	56326.64
5	56315.59	56317.63	56317.78	56305.12	56307.07	56307.14
7	56292.55	56294.70	56295.00	56278.25	56280.26	56280.39
9	56261.63	56263.96	56264.53	56243.64	56245.77	56246.10
11	56223.05	56225.59	56226.35	56201.31	56203.62	56204.15
13	56176.67	56179.49	56180.45	56151.25	56153.79	56154.47
15	56122.51	56125.58	56126.79	56093.41	56096.20	56097.20
17	56060.43	56063.78	56065.21	56027.74	56030.83	56032.04
19	55990.48	55994.48B	55995.85	55954.28	55957.63	55959.09
21	55912.53	55916.52	55918.52	55872.89	55876.55	55878.28
23	55826.52	55830.83	55833.16	55783.58	55787.57C	55789.54
25	55732.37	55737.09	55739.73	55686.24	55690.52	55692.82
27	55629.95	55635.05	55638.09	55580.68	55585.34	55587.99
29	55519.10	55524.71	55528.17	55466.93	55472.03C	55475.01
31				55344.82		

Table 1.15. Wave numbers of the B(15)-X(0) band

N	$R_1(N)$	$R_2(N)$	$R_3(N)$	$P_1(N)$	$P_2(N)$	$P_3(N)$
1	56547.59	56550.41		56544.64		
3	56539.35	56542.22	56542.45	56533.23B	56536.02	56536.62
5	56522.94	56526.00	56526.19	56513.49	56516.41	56516.60
7	56498.40	56501.66	56502.08	56485.59	56488.59B	56488.77B
9	56465.77	56469.29	56469.98	56449.63	56452.82	56453.23
11	56424.98	56428.84	56429.85	56405.43	56408.93	56409.59
13	56376.04	56380.27	56381.60	56353.29	56357.04	56358.01
15	56318.83	56323.47	56325.12	56292.55B	56296.94	56298.27
17	56253.42	56258.44	56260.46	56224.15	56228.75	56230.41
19	56179.49B	56185.11	56187.55	56147.27	56152.27	56154.47B
21	56097.33C	56103.34	56106.20	56062.01	56067.50	56070.13B
23	56006.52	56013.23C	56016.44	55968.37	55974.34	55977.23C
25	55907.05	55914.18	55918.20	55866.18	55872.89B	55876.09
27	55798.82	55806.54	55811.03	55755.36	55762.49	55766.34
29	55681.60C	55689.84	55694.91	55635.78	55643.51	55648.04
31		55564.44	55570.42	55507.31	55515.50	55520.59
33					55378.88	

Table 1.16. Wave numbers of the B(16)-X(0) band

N	$R_1(N)$	$R_2(N)$	$R_3(N)$	$P_1(N)$	$P_2(N)$	$P_3(N)$
1	56714.71	56719.08	56721.78	56712.00		
3	56705.82P	56710.24	56710.54	56700.42B	56704.67	56705.82R
5	56688.34	56692.79	56693.32	56679.99	56684.36	56684.68
7	56662.29	56666.85	56667.77	56650.98	56655.50	56655.88
9	56627.75	56633.28[a]	56634.05	56613.45	56618.01	56618.91
11	56584.68	56590.65	56591.88	56567.43	56572.97[b]	56573.69
13	56533.23B	56539.35B	56541.19	56512.87	56518.82	56520.04
15	56472.65	56479.69	56481.94	56449.63B	56456.18	56457.92
17	56403.56	56411.23	56414.03	56377.94	56384.96	56387.19
19	56325.86	56333.88	56337.51B	56297.43	56305.12B	56307.81B
21	56238.93	56247.72	56251.97	56208.18	56216.38	56219.87
23	56143.05		56157.32	56109.99	56118.70	56122.87
25	56038.02	56047.05	56053.17C	56002.72		56016.97
27	55923.64	55935.72C	55938.61	55886.39	55895.40	55901.47
29	55799.72	55809.85	55819.95?	55760.64	55772.70?	55775.60
31	55666.00	55677.37		55625.40	55635.54C	55645.63C
33	55522.13			55480.42	55491.74	

[a] Perturbed extra line: R(9)= 56632.10
[b] Perturbed extra line: P(11)=56571.77

Table 1.17. Wave numbers of the B(17)-X(0) band

N	$R_1(N)$	$R_2(N)$	$R_3(N)$	$P_1(N)$	$P_2(N)$	$P_3(N)$
1	56845.01	56851.63		56842.52R		
3	56835.46	56842.16	56842.52P	56830.75	56837.34	56838.10
5	56816.84P	56823.82	56824.26	56809.67	56816.27	56816.84R
7	56789.37	56796.63	56797.43	56779.58	56786.42	56786.80
9	56752.88	56760.89	56761.94	56740.52	56747.82	56748.55
11	56707.44	56715.78	56717.69	56692.79B	56700.42B	56701.57
13	56652.99	56661.99B	56664.48	56635.67	56643.99	56645.83
15	56589.46	56598.75	56602.28	56569.75	56578.63	56581.16
17			56530.89	56494.78	56504.09	56507.51
19	56434.79	56443.11	56448.54	56410.62	56419.98	56425.64
21	56343.37	56357.07C	56361.79	56317.27C	56325.54C	56330.95C
23	56242.51	56256.58	56261.60C	56214.36	56228.12	56232.79
25	56131.98	56146.49		56102.16	56116.21	56121.24

Table 2.2. Wave numbers of the B(2)-X(1) band

N	R(N)	R(N)sh	P(N)
3	49153.02		
5	49144.65		49127.32
7	49131.18	49131.81	49107.76
9	49112.65		49082.97
11	49089.20		49053.11
13	49060.20		49018.07

Table 2.3. Wave numbers of the B(3)-X(1) band

N	R(N)	P(N)
1	49796.85	
3	49793.79	49783.38
5	49785.55[a]	49768.44
7	49771.54	49748.42
9	49752.34	49723.16
11	49728.13	49692.71
13	49698.60	49657.05
15	49663.79	49616.23
17	49623.77	49570.01

[a] Overlapped with line from (1,0) band.

Table 2.4. Wave numbers of the B(4)-X(1) band

N	R(N)	P(N)
1	50413.08	
3	50410.86	50400.63
5	50401.71	50386.52R
7	50386.52P	50365.37
9	50367.59	50339.56
11	50342.56	50308.44
13	50312.68	50272.04
15	50276.67	50230.23
17	50235.85	50183.32
19	50189.79	

Table 2.5. Wave numbers of the B(5)-X(1) band

N	R(N)	P(N)
1	51006.25	51002.44R
3	51002.44P	50992.89R
5	50992.89P	50977.40
7	50977.80	50956.70
9	50957.65B	50930.16
11	50931.93	50898.37
13	50900.64	50861.19
15	50863.88	50818.43B
17	50821.63	50770.42
19	50773.90	50716.73
21	50720.54	50657.75
23	50661.69C	50593.13

Table 2.6. Wave numbers of the B(6)-X(1) band

N	R(N)	P(N)
1	51567.51	51563.71R
3	51563.71P	51553.89R
5	51553.89P	51538.32R
7	51538.32P	51517.26R
9	51517.26P	51490.42R
11	51490.42P	51458.18R
13	51458.18P	51420.07R
15	51420.07P	51376.44R
17	51376.44P	
19		51272.26R
21	51272.26P	
23		51145.58R
25	51145.58P	

Table 2.7. Wave numbers of the B(7)–X(1) band

N	R(N)	P(N)
1	52100.95	52096.98R
3	52096.98P	52086.77R
5	52086.77P	52070.92R[a]
7	52070.92P[a]	52049.28R
9	52049.28P	52021.85R
11	52021.85P	51989.01
13	51988.15	51949.95
15		51905.19
17	51903.57	51855.27
19	51852.90	51798.54
21	51796.08	
23		51668.67
25	51655.27	51594.79
27	51591.01	

[a] Overlapped with line from (5,0) band.

Table 2.8. Wave numbers of the B(8)–X(1) band

N	R(N)	P(N)
1	52600.63	52596.36R
3	52596.36P	52585.93R
5	52585.93P	52570.49
7	52569.02	52548.96C
9	52546.39C	52520.53
11	52517.31	52486.61C
13	52483.12C	52447.07
15	52442.62	52400.79
17	52396.12	52348.87
19	52343.37	52291.01
21	52284.89	52227.14
23	52220.11	52157.34
25	52149.08	52082.18

Table 2.9. Wave numbers of the B(9)–X(1) band

N	R(N)	R(N)sh	P(N)	P(N)sh
1	53066.82		53062.20	
3	53061.62		53052.23	
5	53050.32		53036.07	
7	53033.03		53013.36C	
9	53009.36C		52984.67	52985.05B
11	52979.53	52979.95B	52949.70	52950.14B
13	52943.65	52944.13B	52908.61	52909.06B
15	52901.42	52901.94B	52861.43	52861.72B
17	52853.15	52853.60B	52807.87	52808.44B
19	52798.60	52799.20B	52748.35	52748.96B
21	52737.73	52738.32B	52682.39	
23	52670.95		52610.19	
25	52600.39			

Table 2.10. Wave numbers of the B(10)–X(1) band

N	$R_1(N)$	$R_{2,3}(N)$	$P_1(N)$	$P_{2,3}(N)$
1	53495.32		53490.91	
3	53490.09		53481.19	
5	53478.18		53464.39	
7	53459.70		53441.28	
9	53435.40		53411.54	
11	53403.87	53404.42	53375.70	
13	53366.93		53333.38	
15	53322.68	53323.31	53285.20	
17	53272.57	53273.31	53229.36	53229.83
19	53216.48		53167.61	53168.26
21	53152.39	53153.27	53099.80	
23	53082.47	53083.50	53024.88	53025.89
25	53006.24			

Table 2.11. Wave numbers of the B(11)–X(1) band

N	$R_1(N)$	$R_{2,3}(N)$	$P_1(N)$	$P_{2,3}(N)$
1	53882.88		53879.96	
3	53877.86B[a]		53868.93	
5	53865.03		53851.83	
7	53845.64		53828.08	53828.50
9	53820.17		53797.55	
11	53787.76		53760.55	
13	53748.54		53716.83	
15	53702.45		53666.32	
17	53650.26	53651.78	53609.10	
19	53590.71	53592.08	53544.76	
21	53524.70	53526.37	53475.37	
23			53378.29	

[a] Overlapped with a line from the (12,0) band.

Table 2.12. Wave numbers of the B(12)–X(1) band

N	$R_1(N)$	$R_2(N)$	$R_3(N)$	$P_1(N)$	$P_2(N)$	$P_3(N)$
1	54227.89			54224.34		
3	54221.52	54222.45R	54222.45R	54213.65	54214.29	54214.75
5	54208.28	54209.17	54209.31B	54196.09	54196.76	
7	54188.12	54189.10	54189.33B	54171.39	54172.24	
9	54160.88	54162.09		54140.19	54141.34	
11	54126.84	54128.04R	54128.04R	54101.34B	54102.23	
13	54085.88	54087.22	54087.92	54055.95	54057.08	54057.36
15	54037.90			54003.65	54004.86	54005.06
17	53982.90	53984.66	53985.06	53944.32		
19	53920.87	53922.54	53923.38	53877.86	53880.04	
21	53851.83B	53853.96		53804.62	53806.56	53807.13
23				53724.32	53726.78	
25	53692.30	53695.49				

Table 2.13. Wave numbers of the B(13)–X(1) band

N	$R_1(N)$	$R_2(N)$	$R_3(N)$	$P_1(N)$	$P_2(N)$	$P_3(N)$
1	54528.02	54529.33		54524.71		
3	54521.20	54522.45	54522.75	54513.85B	54515.09	54515.57
5	54507.04	54508.41B	54508.84B	54495.64	54497.40PB	54497.40PB
7	54485.66	54487.08	54487.40	54470.10	54471.47	54471.56B
9	54457.00	54458.56	54458.99	54437.37	54438.78	54439.06
11	54421.13	54422.81	54423.39	54397.37	54398.89	54399.32
13	54377.94	54379.79	54380.56	54350.13	54351.78	54352.37
15	54327.48B	54329.49B	54330.42	54295.59	54297.45	54298.50B
17	54269.60	54271.84	54272.95	54233.73	54235.94B	54236.66
19	54204.38	54206.83	54208.26	54164.64	54166.84	54167.91
21	54131.74	54134.39	54135.81	54088.14	54090.60	54091.89
23	54051.59	54054.46	54056.00B	54004.23	54006.86	54008.32
25	53963.83	53966.84	53968.82	53912.81	53915.71	53917.33
27				53813.75	53817.20	

Table 2.14. Wave numbers of the B(14)–X(1) band

N	$R_1(N)$	$R_2(N)$	$R_3(N)$	$P_1(N)$	$P_2(N)$	$P_3(N)$
1		54783.96				
3	54774.76	54776.62	54776.83	54768.02	54769.78	54770.80
5	54759.64	54761.61	54761.86	54749.17	54750.99	54751.16
7	54736.95	54739.04	54739.43	54722.72	54724.70	54724.84
9	54706.66	54708.93	54709.49	54688.63	54690.78	54691.10
11	54668.72	54671.25	54672.03	54646.98	54649.32	54649.72
13	54623.13B	54625.95	54626.93	54597.71	54600.25	54600.96
15	54569.80	54572.96	54574.16	54540.78	54543.56	54544.54
17	54508.84B	54512.22	54513.85B	54476.24	54479.26	54480.49
19	54440.13	54443.76	54445.48	54403.98	54407.27	54407.70
21	54363.48	54367.44	54369.47	54323.88	54327.48B	54329.49B
23	54278.86	54283.20	54285.59	54235.94B	54239.91	54241.95
25	54186.34	54191.10	54193.77	54140.19B	54114.44	54146.97
27	54085.88B	54090.60B	54093.26	54036.60	54040.94	54043.61
29					53929.56	53932.52

Table 2.15. Wave numbers of the B(15)-X(1) band

N	$R_1(N)$	$R_2(N)$	$R_3(N)$	$P_1(N)$	$P_2(N)$	$P_3(N)$
1						
3	54983.04	54986.03R	54986.03R	54976.96	54979.40B	54980.16
5		54970.06R	54970.06R			
7	54942.85	54946.13	54946.51	54930.09B	54933.10P	54933.10P
9	54910.70	54914.21	54914.94	54894.50	54897.72	54898.12
11	54870.64	54874.46	54865.46	54851.04	54854.54	54855.20
13	54822.39	54826.53	54827.97	54799.61	54803.43	54804.43
15	54766.15	54770.80B	54772.48	54740.10	54744.29	54745.58
17	54701.77	54706.66B	54708.93B	54672.52	54677.13	54678.78
19	54629.13	54634.69	54637.10	54596.83	54601.88	54603.91
21	54548.23	54554.25	54557.08	54512.93	54518.45	54520.92
23	54458.99B	54465.50	54468.87	54420.82	54426.70	54429.58
25	54360.93	54368.06	54371.99	54320.12	54326.65	54330.42B
27	54254.46	54262.22				

Table 2.16. Wave numbers of the B(16)-X(1) band

N	$R_1(N)$	$R_2(N)$	$R_3(N)$	$P_1(N)$	$P_2(N)$	$P_3(N)$
1	55158.30					
3	55149.54B	55153.96	55154.34	55144.04	55148.30	55149.54R
5	55132.31	55136.81	55137.23	55123.96	55128.31	55128.70
7	55106.67	55111.20	55112.15	55095.37B	55099.88	55100.34
9	55072.62	55078.21	55078.97	55058.38	55062.94	55063.86
11	55030.22	55037.34R	55037.34R	55013.02	55018.60	
13	54979.40B	54985.87	54987.58	54958.79B	54965.21	54966.64B
15	54920.63B	54926.97	54930.09B	54897.05	54903.47	54905.20
17	54851.97	54859.56	54862.41	54826.37	54833.30	54835.59
19	54775.25	54783.50	54787.02	54747.00	54754.58	54757.40
21	54689.78	54698.56	54702.77	54659.02	54667.25	54671.25B
23	54595.40	54604.53		54562.29	54571.01	54575.19

Table 2.17. Wave numbers of the B(17)-X(1) band

N	$R_1(N)$	$R_2(N)$	$R_3(N)$	$P_1(N)$	$P_2(N)$	$P_3(N)$
1	55288.60	55292.23		55286.14R		
3	55279.26	55285.90	55286.14P	55274.33B	55280.89	
5	55260.78P	55267.15	55268.33	55253.64	55260.27	55260.78R
7	55233.70	55241.15	55241.73	55223.96	55230.88	55231.25
9	55197.79	55205.58	55206.88	55185.39	55192.66	55193.52
11	55153.02	55161.25B	55163.07	55138.10	55145.97	55147.19
13	55099.45	55108.26	55110.87	55082.02	55090.33	55092.19
15		55046.20B	55049.56B	55016.91?	55025.86	55028.63
17	54965.21B	54974.47	54979.40B	54943.03	54952.46	54955.87
19	54884.34	54892.70	54898.12B	54860.19	54869.50	54875.81
21	54794.23	54807.90	54812.67	54768.02B	54776.62B	
23	54694.85	54708.93B		54666.68	54680.36	54685.07
25	54585.23	54600.25B		54556.06		54575.19B

Table 3. Wave numbers of observed lines near the dissociation limit

Present		Brix and Herzberg[7]	
Line	Assignment[a]	Line	Assignment[b]
57130.80		57130.73	n,PXi3(1)
57130.02?			
57129.51		57129.50	n,Ri(1)
57129.13?			
57128.68		57128.65	
57128.30			
57123.06?			
57122.00			
57120.94			
57119.14			
57117.59D		57117.70	
57117.14			
57116.77		57116.82	n,Ri(3)
57115.69		57115.72	
57115.22		57115.30	n,Pi(3)
57114.66			
57114.29		57114.36	21,RP31(1)
57113.44B			
57113.15			
57112.76		57112.98	21,R2(1)
57112.27		57112.25	21,RQ32(1)
57111.27?			
57109.02			
57108.61		57108.73	
57107.72			
57106.47			
57106.00			
57105.45			
57103.56		57103.68	
57102.85B			
57102.35D		57102.36	21,R3(3)
57101.65D		57101.58	
57101.00DB			
57100.58		57100.55	21,R2(3)
57100.42B			
57099.97		57100.01	21,P3(3)
57098.99D		57099.00	
57098.41		57098.41	21,P2(3)
57095.66D		57095.69	
57094.57			
57093.78D		57093.88	
57093.34		57093.30	n,Ri(5)
57092.69		57092.58	
57092.41B			
57091.79		57091.81	
57091.11B			
57090.98		57091.04	n,Pi(5)
57089.75		57089.78	
57087.83B			
57087.34		57087.36	
57086.12			
57085.63		57085.64	
57084.71		57084.76	
57083.97		57083.94	
57083.10		57082.92	20,RQ21(1)
57082.75D			
57082.17D		57082.22	20,RP31(1)
57081.64B			
57081.20D		57081.20	20,R2(1)
57080.12		57080.14	21,R3(5);20,RQ32(1)
57079.56		57079.59	
57078.14		57078.17	21,R2(5)
57077.59D			
57076.98B			
57076.50		57076.46	21,P3(5)
57076.11B		57076.16	
57074.77		57074.80	21,P2(5)
57073.64?			
57073.37B?			
57072.99		57073.00	
57072.44			
57071.99		57072.00	20,R3(3)
57070.64?B			
57070.17?B			
57069.68		57069.68	20,R2(3)
57068.92D			
57067.94B			
57067.69D		57067.69	20,P3(3)
57067.36			
57066.78		57066.82	20,P2(3)
57065.94		57065.94	
57064.44?		57064.21B	
57063.87		57063.91	
57061.47D			
57059.41D			
57058.92		57058.94	
57057.96		57057.95	
57056.80		57056.78	
57056.39?			
57055.95		57055.93	n,Pi(7)
57055.27D		57055.24	
57055.13B			
~~57054.48~~		~~57054.50~~	
57053.92B			
57053.43		57053.42	
57052.51		57052.56	
57051.99		57051.94	
57051.09		57051.09	
57050.47		57050.44	20,R3(5)
57049.90			
57049.13D			
57048.31		57048.26	20,R2(5)
57047.20		57047.12	21,R3(7)
57046.86B		57046.84	
57046.04		57046.02	20,P3(5)
57045.19		57045.14	21,R2(7)
57043.83		57043.80	20,P2(5)
57043.35			
57042.67		57042.67	21,P3(7)
57042.13		57042.14	
57041.26			
57040.76		57040.78	21,P2(7)
57040.12			
57039.52			
57038.99		57038.83	
57038.68B			
57037.25			
57036.57		57036.53	
57035.20D		57035.21	
57034.78D		57034.78	
57034.17		57034.14	
57033.46B			
57033.08			
57032.77		57032.85	19,TR31(1)
57031.56D			
57030.97		57030.91	19,RQ21(1)
57029.98		57029.88	19,RP31(1)
57029.79B			
57028.98B			
57028.84		57028.07	19,R2(1)
57027.85		57027.80	19,RQ32(1)
57026.53		57026.48	
57025.30B			
57024.76		57024.69	
57023.67		57023.62	19,TR31(3)
57022.58B			
57022.40		57022.26	
57022.05			
57021.42B			
57020.95		57020.90	
57020.04		57019.99	19,RQ21(3)
57019.19		57019.10	20,R3(7)
57018.53		57018.41	19,R3(3)
57018.13		57018.09	19,R2(3)
57016.92		57016.83	20,R2(7)
57016.47		57016.47	19,R1(1)+PR13(1)+PQ23(3)
57015.55		57015.57	19,P3(3)
57014.94B			
57014.55		57014.52	19,P2(3)+P1(1)
57013.68B			
57013.04		57013.01	20,P3(7)
57011.79			
57011.34B			
57010.91		57010.89	20,P2(7);19,TR31x(5)
57009.73		57009.62	
57009.22D		57009.14	
57007.83			
57007.03			
57006.30B			
57005.66		57005.61	19,R1(3)

Table 3. Wave numbers of observed lines near the dissociation limit --Continued

Present		Brix and Herzberg[7]	
Line	Assignment[a]	Line	Assignment[b]
57005.02		57004.95	19,TR31(5)
57004.27		57004.15	21,R3(9)
57003.66			
57003.26			
57002.84		57002.90	
57002.14		57002.11	19,P1(3)
57001.56		57001.62	21,R2(9)
57000.63			
57000.29		57000.12	19,NP13(3)+PQ12(3)
56999.93			
56998.87		56998.90	
56998.36		56998.27	21,P3(9)
56997.85		56997.80	19,R2(5)+R3(5)
56996.80		56996.77	
56996.32		56996.30	21,P2(9)
56995.87B			
56994.18D			
56993.59			
56992.59		56992.55	19,P3(5)+P2(5)
56992.24			
56991.38B		56991.33	
56990.70D		56990.65	
56989.89		56989.85	
56988.08			
56986.86D			
56985.94			
56985.61		56985.92	
56985.09		56985.04	19,R1(5)
56984.32B		56984.23	
56982.72		56982.77	
56982.22			
56981.62			
56981.14			
56979.81		56979.76	19,P1(5)
56979.03		56979.03	
56978.03		56977.96	20,R3(9)
56977.74B			
56977.27			
56976.35		56976.29	19,NP13(5)+TR31x(7)
56975.56		56975.48	20,R2(9)
56974.07		56974.03	
56973.57		56973.45	19,R3x(7)
56973.08?			
56972.36		56972.23	
56972.20B		56972.23	
56971.42		56971.39	
56970.32		56970.26	20,P3(9)
56968.65			
56968.08			
56967.70		56967.82	19,R3(7)+R2(7);20,P2(9)
56966.30B		56966.79	19,P3x(11)
56965.86		56965.80	
56964.54		56964.52	
56963.93			
56962.42			
56961.18		56961.13	
56960.48		56960.40	19,P3(7)+P2(7)
56959.84		56959.71	
56958.14D		56958.09	18,TR31(1)
56957.20		56957.16	
56955.84B			
56955.27B			
56954.75		56954.60	19,R1(7);18,RP31(1)
56954.02		56953.97	
56953.52		56953.46	18,R2(1)
56952.52		56952.46	18,RQ32(1)
56951.60D		56951.40	
56950.33		56950.13	18,TR31(3)
56949.96			
56948.97		56948,88	
56948.38?B			
56947.76		56947.63	19,P1(7);21,R2(11)
56946.01B			
56945.61		56945.51	
56944.77B			
56943.99			
56943.89		56943.76	18,R3(3)+R1(1)+PR13(1)
56943.26		56943.22	18,R2(3);21,P3(11)
56942.46		56942.40	19,NP13(7)
56941.76		56941.68	18,P1(1)

Table 3. Wave numbers of observed lines near the dissociation limit --Continued

Present		Brix and Herzberg[7]	
Line	Assignment[a]	Line	Assignment[b]
56941.35B		56941.32	21,P2(11);18,PQ23(3)
56940.22		56940.19	18,P3(3)
56939.15		56939.05	18,P2(3)
56938.79		56938.77	
56937.60		56937.50	
56937.22B			
56936.41D		56936.32	
56934.38B			
56933.89		56933.78	18,R1(3)
56932.97		56932.96	
56932.29		56932.22	19,R3(9)
56931.10		56931.08	
56930.28B			
56929.66		56929.56	18,P1(3)
56928.66		56928.46	19,R2(9)
56928.41B			
56927.52		56927.44	18,NP13(3)+PQ12(3);19,R3x(9)
56926.78		56926.68	20,R3(11)
56925.50B			
56924.49			
56924.22		56924.22	18,R3(5);19,P3x(9);20,R2(11)
56923.61		56923.53	18,R2(5)
56922.56		56922.47	
56919.30		56919.19	19,P2(9)
56918.73		56918.64	19,P3(9)
56917.96			
56917.71		56917.61	18,P3(5)+P2(5);20,P3(11)
56917.42			
56915.20		56915.11	20,P2(11)
56914.57		56914.48	18,R1(5);19,R1(9)
56910.73			
56909.46		56909.38	18,R1x(5)
56908.13		56908.01	18,P1(5)
56906.42			
56905.92		56905.88	19,P1(9)
56904.44			
56903.77D		56903.78	18,NP13(5)
56902.64		56902.54	
56901.34		56901.31	
56900.88		56900.80	
56899.48			
56898.98		56898.93	19,NP13(9)
56896.75B			
56896.19		56896.12	18,R3(7)
56894.64		56894.60	18,R2(7)
56891.34			
56891.06		56891.08	
56890.76			
56889.83		56889.74	
56888.73		56888.64	
56887.19B			
56887.09		56887.00	18,P3(7)
56886.27		56886.26	18,P2(7)
56885.09D		56885.02	
56883.31			
56883.10		56883.09	18,R1(7);19,R3(11)
56881.52			
56880.75			
56879.62		56879.54	19,R2(11)
56878.78			
56878.08			
56877.19		56877.11	18,P1(7)
56875.81B			
56875.58		56875.54	21,P2(13)
56872.46		56872.37	
56872.04		56871.95	19,P3(11);18,P1x(7)
56871.09			
56870.63		56870.60	18,NP13(7)
56868.80?			
56868.41		56868.32	19,P2(11)
56867.06			
56866.55		56866.79	19,P3x(11)
56865.21B			
56865.06		56865.02	19,R1(11)
56863.89			
56863.38		56863.35	
56862.47		56862.32	
56861.14		56861.17	
56860.32		56860.34	
56860.17B			

Table 3. Wave numbers of observed lines near the dissociation limit --Continued

Present		Brix and Herzberg[7]	
Line	Assignment[a]	Line	Assignment[b]
56859.34			
56858.79		56858.74	
56856.80?			
56856.55	17,TR31(1)	56856.49	17,TR31(1)
56856.01		56855.96	18,R2(9)
56854.94		56854.85	20,P3(13)
56854.39		56854.33	19,P1(11);17,R3(1)
56853.55	17,RQ21(1)	56853.45	17,RQ21(1)
56852.33	17,RP31(1)	56852.22	17,RP31(1);20,P2(13)
56851.63	17,R2(1)	56851.58	17,R2(1)
56850.55	17,RQ32(1)	56850.40	17,RQ32(1)
56850.24B	17,TR31(3)	56850.14	17,TR31(3)
56847.87			
56847.33		56847.24	18,P3(9)
56846.35		56846.27	18,R1(9)
56845.76		56845.66	18,P2(9)
56845.01	17,R1(1)	56844.85	17,R1(1)+PR13(1)
56844.75B	17,PR13(1)		
56843.82			
56843.55B			
56842.52	17,R3(3)+P1(1)	56842.30	17,R3(3)+R2(3)+P1(1)
56842.16	17,R2(3)		
56840.44	17,PQ12(1)+PQ32(3)	56840.44	17,PQ12(1)
56839.37	17,PQ23(3)	56839.36	17,PQ23(3)
56838.10	17,P3(3)	56838.15	17,P3(3)
56837.54B			
56837.34	17,P2(3)	56837.33	17,P2(3);18,P1x(9)
56836.43			
56835.46	17,R1(3)	56835.45	17,R1(3)
56835.00B	17,TR31(5)		
56834.50		56834.50	17,TR31(5);18,P1(9)
56833.61			
56833.06			
56831.36B			
56830.75	17,P1(3)	56830.70	17,P1(3)
56829.80			
56828.81B	17,PQ12(3)		
56828.37	17,NP13(3)	56828.22	17,NP13(3)
56827.58			
56825.57B			
56825.03			
56824.26	17,R3(5)		
56823.82	17,R2(5)	56824.02	17,R2(5)+R3(5)
56822.23			
56820.81		56820.71	19,R2(13)
56819.36			
56816.84	17,R1(5)+P3(5)	56816.57	17,R1(5)+P3(5)+P2(5)
56816.27	17,P2(5)		
56815.15			
56813.00			
56812.05			
56811.24		56811.16	19,P3(13)
56809.67	17,P1(5)	56809.62	17,P1(5)
56807.98B			
56807.72		56807.70	19,P2(13)
56806.64D			
56805.01B	17,NP13(5)	56804.99	19,R1(13);17,NP13(5)
56801.56W			
56800.71B			
56800.18			
56798.34		56798.14	18,R1(11)+P3(11)
56797.43	17,R3(7)	56797.35	17,R3(7)
56796.63	17,R2(7)	56796.63	17,R2(7)
56796.20B			
56795.65		56795.58	18,P2(11)
56794.42			
56793.86			
56793.17		56793.03	19,P1(13)
56792.98B			
56792.49			
56791.68			
56790.87			
56790.34			
56790.04?			
56789.37	17,R1(7)	56789.26	17,R1(7)

Table 3. Wave numbers of observed lines near the dissociation limit --Continued

Present		Brix and Herzberg[7]	
Line	Assignment[a]	Line	Assignment[b]
56788.91			
56788.37			
56786.80	17,P3(7)		
56786.42	17,P2(7)	56786.51	17,P3(7)+P2(7);18,P1(11)
56786.16B			
56784.71?			
56783.41D			
56782.69			
56782.53		56782.45	19,NP13(13)
56781.99			
56781.24			
56780.03			
56779.58	17,P1(7)	56779.63	17,P1(7)
56778.06D	17,TR31(9)	56778.03	17,TR31(9)
56776.87		56776.76	18,NP13x(11)
56776.18			
56775.29			
56774.41B?			
56774.20			
56773.05?			
56772.37	17,NP13(7)	56772.28	17,NP13(7)
56770.72?			
56768.67			
56766.98			
56764.16			
56761.94	17,R3(9)	56761.86	17,R3(9)
56761.14			
56760.89	17,R2(9)	56760.84	17,R2(9)
56759.74			
56756.42			
56755.91			
56755.73B			
56754.19?			
56753.45D?			
56752.88	17,R1(9)	56752.82	17,R1(9)
56752.51B?			
56749.66			
56748.55	17,P3(9)	56748.43	17,P3(9)
56747.82	17,P2(9)	56747.81	17,P2(9)
56746.53			
56741.37B			
56741.14			
56740.52	17,P1(9)	56740.50	17,P1(9)
56738.01			
56737.56		56737.70	19,P2(15)
56736.90?			
56736.31			
56735.77		56735.62	19,R1(15)
56735.59B			
56734.47?			
56733.43			
56731.91			
56731.16B?			
56730.65	17,NP13(9)	56730.57	17,NP13(9)
56730.15?			
56730.00			
56728.74B			
56728.33			
56726.45		56726.32	18,P1(13)
56725.71			
56724.93	16,TR31(1)	56724.48	16,TR31(1)
56724.41B			
56722.54			
56721.78	16,R3(1)	56721.72	16,R3(1);19,P1(15)

[a] See the text (sec. 3.2.4).
[b] In this column the upper state vibrational quantum number is followed by the rotational line assignment written, for convenience, without subscripts or superscripts.

Table 4. Wave numbers of satellite and forbidden lines calculated from term values[a]

B(9)–X(0) band

N	${}^{P}R_{13}(N)$	${}^{P}Q_{12}(N)$	${}^{P}Q_{23}(N)$	${}^{R}Q_{21}(N)$	${}^{R}Q_{32}(N)$	${}^{R}P_{31}(N)$	${}^{T}R_{31}(N)$	${}^{N}P_{13}(N)$
1	54620.49	54616.55		54626.34				
3	54608.76	54606.69	54612.18	54620.23				54604.26
5	54592.03	54590.01	54594.42	54608.66				54582.82
7	54568.96	54566.98	54571.28	54590.89				54554.62
9	54539.60	54537.65	54541.97	54566.75				54520.07

B(10)–X(0) band

N	${}^{P}R_{13}(N)$	${}^{P}Q_{12}(N)$	${}^{P}Q_{23}(N)$	${}^{R}Q_{21}(N)$	${}^{R}Q_{32}(N)$	${}^{R}P_{31}(N)$	${}^{T}R_{31}(N)$	${}^{N}P_{13}(N)$
1	55049.43	55045.49		55055.64				
3	55037.41	55035.35	55041.47	55048.18				55033.20
5	55020.29	55018.27	55022.37	55035.98				55011.47
7	54996.67	54994.69	54998.60	55017.57				54982.88
9	54966.35	54964.40	54968.65	54992.48				54947.78

B(11)–X(0) band

N	${}^{P}R_{13}(N)$	${}^{P}Q_{12}(N)$	${}^{P}Q_{23}(N)$	${}^{R}Q_{21}(N)$	${}^{R}Q_{32}(N)$	${}^{R}P_{31}(N)$	${}^{T}R_{31}(N)$	${}^{N}P_{13}(N)$
1	55437.36	55433.42		55441.84				
3	55425.15	55423.09	55427.67	55435.82				55421.13
5	55407.74	55405.72	55410.01				55439.20	55399.21
7	55383.54	55381.56		55403.41	55399.84	55401.85		55370.33
9	55352.23	55350.28	55354.49	55377.23				55334.65

B(12)–X(0) band

N	${}^{P}R_{13}(N)$	${}^{P}Q_{12}(N)$	${}^{P}Q_{23}(N)$	${}^{R}Q_{21}(N)$	${}^{R}Q_{32}(N)$	${}^{R}P_{31}(N)$	${}^{T}R_{31}(N)$	${}^{N}P_{13}(N)$
1	55782.69 55782.85	55778.75		55786.83 55786.96	55783.37 55783.61	55785.25	55792.82	
3	55770.02	55767.95	55772.66 55772.68	55780.49	55776.59	55778.53	55791.00	55766.46 55766.27
5	55751.95	55749.94	55754.68 55754.71	55766.99	55763.17	55765.16	55782.14	55744.07
7	55726.83	55724.85	55729.61	55746.54	55742.78	55744.79	55766.12	55714.54
9	55694.67	55692.72	55697.61	55718.97	55715.25	55717.29	55743.11	55677.94

B(13)–X(0) band

N	${}^{P}R_{13}(N)$	${}^{P}Q_{12}(N)$	${}^{P}Q_{23}(N)$	${}^{R}Q_{21}(N)$	${}^{R}Q_{32}(N)$	${}^{R}P_{31}(N)$	${}^{T}R_{31}(N)$	${}^{N}P_{13}(N)$
1	56083.12 56083.14	56079.18		56087.55 56087.55	56084.16 56084.26	56086.04 56086.03	56093.13	
3	56070.24	56068.17 56068.14	56073.39 56073.32	56080.63	56076.90	56078.84	56090.33 56090.38	56066.89 56066.83
5	56051.60	56049.59 56049.59	56054.82 56054.78	56066.37 56066.26	56062.50	56064.49	56080.34	56044.30 56044.29
7	56025.60	56023.62	56028.99	56044.64 56044.78	56040.98	56042.99	56062.96	56014.19
9	55992.25	55990.30	55995.72	56015.58	56012.09	56014.13	56038.18	55976.71

B(14)–X(0) band

N	${}^{P}R_{13}(N)$	${}^{P}Q_{12}(N)$	${}^{P}Q_{23}(N)$	${}^{R}Q_{21}(N)$	${}^{R}Q_{32}(N)$	${}^{R}P_{31}(N)$	${}^{T}R_{31}(N)$	${}^{N}P_{13}(N)$
1	56337.48 56337.51	56333.54		56342.32 56342.30	56338.93 56338.93	56340.81 56340.78B	56347.25 56347.35	
3	56324.43	56322.36 56322.27	56328.15 56328.11	56334.86 56334.84	56331.02	56332.96	56343.60 56343.85?	56321.25 56321.22
5	56305.16	56303.15	56309.05 56309.00	56319.62 56319.54	56315.78	56317.76	56332.38	56298.48 56298.27B
7	56278.21	56276.23	56282.24	56296.68	56293.02	56295.03	56313.44	56267.75 56367.79
9	56243.59	56241.64	56247.75	56266.00	56262.57	56264.61	56286.78	56229.32 56229.29

B(15)–X(0) band

N	${}^{P}R_{13}(N)$	${}^{P}Q_{12}(N)$	${}^{P}Q_{23}(N)$	${}^{R}Q_{21}(N)$	${}^{R}Q_{32}(N)$	${}^{R}P_{31}(N)$	${}^{T}R_{31}(N)$	${}^{N}P_{13}(N)$
1	56546.70 56546.73	56542.76		56552.27 56552.26B	56548.91 56549.05	56550.79 56550.84B	56556.66 56556.70	
3	56533.39	56531.32 56531.30	56538.11 56538.10	56544.20	56540.43 56540.31	56542.37	56552.00 56552.26B	56530.47 56530.53
5	56513.53	56511.51	56518.39	56527.97	56524.17 56524.26	56526.16	56539.48 56539.44B	56507.45 56507.56B
7	56485.56	56483.58	56490.59 56490.58?	56503.68	56500.12 56500.19?	56502.13	56518.89	56476.12 56476.10
9	56449.51	56447.56	56454.76	56471.32	56468.02	56470.06	56490.30	56436.67 56436.74

Table 4. Wave numbers of satellite and forbidden lines calculated from term values[a] --Continued

B(16)–X(0) band

N	$^{P}R_{13}(N)$	$^{P}Q_{12}(N)$	$^{P}Q_{23}(N)$	$^{R}Q_{21}(N)$	$^{R}Q_{32}(N)$	$^{R}P_{31}(N)$	$^{T}R_{31}(N)$	$^{N}P_{13}(N)$
1	56714.06	56710.12		56720.93	56717.97	56719.85	56724.75	
	56714.13			56720.95		56719.62	56724.93	
3	56700.55	56698.48	56706.77	56712.18	56708.51	56710.45	56719.12	56697.83
		56698.26			56708.66		56719.11R	56697.85
5	56680.01	56678.00	56686.37	56694.82	56691.29	56693.28	56705.17	56674.60
		56677.87			56691.60?			56674.72
7	56650.95	56648.97	56657.44	56668.87	56665.81	56667.82	56682.97	56642.60
							56683.05	56642.65
9	56613.36	56611.41	56619.95	56635.33	56632.10	56634.14	56652.33	56602.06

B(17)–X(0) band

N	$^{P}R_{13}(N)$	$^{P}Q_{12}(N)$	$^{P}Q_{23}(N)$	$^{R}Q_{21}(N)$	$^{R}Q_{32}(N)$	$^{R}P_{31}(N)$	$^{T}R_{31}(N)$	$^{N}P_{13}(N)$
1	56844.58	56840.64		56853.54	56850.39	56852.27	56856.82	
	56844.75B	56840.44B		56853.55	56850.55	56852.33	56856.55	
3	56830.86	56828.79	56839.38	56844.10	56840.58	56842.52	56850.05	56828.35
		56828.81B	56839.37		56840.44B		56850.24B	56828.37
5	56809.67	56807.66	56818.29	56825.79	56822.22	56824.21	56834.82	56804.92
							56835.00B	56805.01B
7	56779.50	56777.52	56788.41	56798.67	56795.46	56797.47	56810.86	56772.26
								56772.37
9	56740.44	56738.49	56749.74	56762.86	56759.99	56762.03	56778.13	56730.61
							56778.06	56730.65

[a] Where a pair of wave number values is given for a line the upper and lower entries are the calculated and observed values, respectively. Where a single value is given it is the calculated value. See the text(sec. 3.2.5).

3.2.2. Photographic Atlas

In Figs. 1–18, we present a photographic atlas of the Schumann–Runge absorption bands of O_2 at 300 K in the wavelength region 205–175 nm. Each of the figures, except those (Figs. 1 and 2) for the weak (0,0) and (1,0) bands, shows the spectrum at two pressures chosen for optimal presentation of strong and weak absorption lines against a vacuum wavelength scale in nanometers. The emission lines seen belong to CO (Sec. 3.2.1). The rotational assignments of the principal branches of the bands (v',0) with $v' = 0$–21 are shown in Figs. 1–18 and of the bands (v',1) with $v' = 2$–16 in Figs. 1–11.

3.2.3. Principal Rotational Branches of the B(v')–X(0) and B(v')–X(1) Bands

The measured line positions and rotational assignments of the principal branches of the bands (v',0) with $v' = 0$–17 are given in Tables 1.0–1.17 and of the bands (v',1) with $v' = 2$–17 in Tables 2.2–2.17; no previous high resolution results for the (v',1) bands are available.

For lines of the (14,0) band (Fig. 15), which are among the sharpest in the Schumann–Runge absorption system, our photographic measurements (Table 1.14) show that all the triplet components are resolved, whereas Brix and Herzberg[7] have resolved $P_2(N)$ from $P_3(N)$ and $R_2(N)$ from $R_3(N)$ only for $N \geqslant 11$. Thus, our photographic resolution is a little better than that of Brix and Herzberg.[7] We have also been able, for some bands, to follow the rotational lines to higher rotational quantum numbers.

With sufficient spectroscopic resolution, the possibility of observing the individual triplet components depends on the extent of their mutual overlapping and that, in turn, depends on the magnitude of the triplet splittings and of the linewidths arising from predissociation in the upper state. For $v' \geqslant 13$, the triplet splittings, which increase with v', are large enough and the predissociation linewidths small enough for the triplet structure to be resolved well in our absorption spectra (Figs. 14–18 and Tables 1.13–1.17 for $v'' = 0$; Figs. 10 and 11 and Tables 2.13–2.17 for $v'' = 1$). For $v' = 1,2,7,9$–12 partial resolution is achieved (Figs. 2, 3, 8, 10–13 and Tables 1.1, 1.2, 1.7, 1.9–1.12 for $v'' = 0$; Figs. 1, 5, 7–9 and Tables 2.2, 2.9–2.12 for $v'' = 1$). For $v' = 0,3$–6,8, where for $v' = 4$–6, the overlapping of R(N) and P($N-2$) is an additional hindrance, the triplet structure is unresolved (Figs. 1, 4–7, 9 and Tables 1.0, 1.3–1.6, 1.8 for $v'' = 0$ and Figs. 2–6, 8 and Tables 2.3–2.6, 2.8 for $v'' = 1$). The partially resolved triplet structures, each consisting of a peak and a less intense blended shoulder at slightly higher wave number, measured for the (1,0), (2,0), and (7,0) bands (Tables 1.1, 1.2, and 1.7) have not been reported previously.

Our rotational assignments of the (v',0) bands are generally in agreement with those of Ackerman and Biaumé[31] and Brix and Herzberg,[7] and we achieve better separation of the triplet structure except for $v' = 0,3$–6,8 when spectroscopic resolution is probably not the limiting factor. However, in the bands (9,0)–(13,0) the $R_3(1)$ lines, which are weak, have been misassigned by Ackerman and Biaumé.[31]

3.2.4. Region Near the Dissociation Limit

In Table 3, we compare all the lines, most of which are sharp, that we have measured from the dissociation limit to the head of the (16,0) band with those of Brix and Herzberg.[17] Our assignments, apart from identifying the (16,0) bandhead, are given only for the (17,0) band, and those of Brix and Herzberg[7] are collected from their Table Ia for the (17,0)–(19,0) bands and from their Table Ib. Because of the presence of perturbations, their rotational assignments of the (17,0)–(19,0) bands extend to only moderate N values, and their assignments of the (20,0) and (21,0) bands are more

Table 5. Term values (cm^{-1}) of the B state of O_2

v' = 9

N	$T_1(N)$	$T_2(N)$	$T_3(N)$
0	54619.43		
2	54623.93	54627.35	
4	54633.14	54635.53	
6	54647.48	54649.80	
8	54667.02	54669.39	
10	54691.70	54694.08	
12	54721.59	54724.00	
14	54756.60	54759.18	
16	54796.72	54799.27	54797.74
18	54841.96	54844.55	54843.11
20	54892.23	54895.07	54893.66
22	54947.73	54950.45	54949.05
24	55008.32	55010.97	55009.76
26	55073.70		
28	55144.04	55147.57	
30	55219.44	55222.82	55222.15

v' = 10

N	$T_1(N)$	$T_2(N)$	$T_3(N)$
0	55048.37		
2	55052.59	55056.64	
4	55061.40	55063.48	
6	55075.20	55077.12	
8	55093.77	55096.07	
10	55117.43	55119.81	
12	55146.03	55148.49	
14	55179.54	55182.13	
16	55217.98	55220.79	
18	55261.25	55264.20	55262.75
20	55309.48	55312.45	55310.92
22	55362.45	55365.60	55364.32
24	55420.24	55423.49	55422.30
26	55482.71	55486.10	55484.87
~~28~~	~~55549.84~~	~~55553.20~~	~~55552.08~~
30	55621.60	55625.08	
32	55697.91	55701.58	55700.85

v' = 11

N	$T_1(N)$	$T_2(N)$	$T_3(N)$
0	55436.30		
2	55440.33	55442.84	
4	55448.85	55451.12	
6	55462.07		
8	55479.65	55481.90	55480.35
10	55502.10	55504.55	
12	55529.24	55531.86	
14	55561.14	55563.91	
16	55597.62	55600.43	55598.86
18	55638.83	55642.01	
20	55684.47	55687.91	55686.49
22	55734.78	55738.28	55736.94
24	55789.76	55793.26	
26			
28	55912.30	55916.25	55915.74

v' = 12

N	$T_1(N)$	$T_2(N)$	$T_3(N)$
0	55781.63		
2	55785.19	55787.84	55786.26
4	55793.07	55795.80	55793.83
6	55805.35	55808.13	55806.30
8	55822.08	55825.03	55823.28
10	55843.22	55846.30	55844.61
12	55868.80	55872.08	55870.43
14	55898.80	55902.17	55900.77
16	55933.08	55936.64	55935.27
18	55971.71	55975.41	55974.19
20	56014.65	56018.43	56017.37
22		56065.71	56064.64
24	56113.10	56117.32	56116.52
26	56168.47	56172.44	56171.82

Table 5. Term values (cm^{-1}) of the B state of O_2 --Continued

v' = 13

N	$T_1(N)$	$T_2(N)$	$T_3(N)$
0	56082.06		
2	56085.41	56088.56	56087.04
4	56092.72	56095.93	56094.14
6	56104.12	56107.52	56105.63
8	56119.66	56123.14	56121.48
10	56139.31	56142.91	56141.45
12	56163.08	56166.82	56165.50
14	56190.87	56194.81	56193.66
16	56222.69	56226.86	56225.85
18	56258.46	56262.81	56262.03
20	56298.14	56302.67	56302.30
22	56341.91	56346.49	56346.28
24	56389.08	56394.14	56394.02
26	56440.12	56445.45	56445.57

v' = 14

N	$T_1(N)$	$T_2(N)$	$T_3(N)$
0	56336.42		
2	56339.60	56343.32	56341.81
4	56346.28	56350.17	56348.26
6	56356.74	56360.76	56358.91
8	56371.00	56375.17	56373.52
10	56388.96	56393.32	56391.94
12	56410.69	56415.29	56414.10
14	56436.09	56440.98	56440.09
16	56465.14	56470.33	56469.69
18	56497.77	56503.24	56502.84
20	56533.91	56539.73	56539.61
22	56573.52	56579.70	56579.86
24	56616.49	56622.97	56623.48
26	56662.62	56669.51	56670.38
28	56711.86	56719.18	56720.43
30	56764.03	56771.86	56773.56

v' = 15

N	$T_1(N)$	$T_2(N)$	$T_3(N)$
0	56545.64		
~~2~~	~~56548.56~~	~~56553.28~~	~~56551.79~~
4	56554.64	56559.50	56557.67
6	56564.08	56569.11	56567.30
8	56576.92	56582.18	56580.63
10	56593.09	56598.64	56597.38
12	56612.68	56618.54	56617.62
14	56635.34	56641.74	56641.20
16	56661.50	56668.23	56668.04
18	56690.76	56697.90	56698.15
20	56722.98	56730.70	56731.39
22	56758.32	56766.49	56767.54
24	56796.46	56805.36	56806.76
26	56837.30	56846.63	56848.79
28	56880.72	56890.67	56893.41
30	56926.52	56936.97	56940.29
32		56985.89	56990.12

v' = 16

N	$T_1(N)$	$T_2(N)$	$T_3(N)$
0	56713.00		
2	56715.72	56721.94	56720.86
4	56721.13	56727.49	56725.75
6	56729.48	56735.96	56734.42
8	56740.78	56747.37	56746.31
0	56755.08	56762.66	56761.47
2	56772.32	56780.33	56779.65
4	56792.48	56800.90	56800.82
6	56815.31	56824.45	56824.84
8	56840.91	56850.72	56851.61
20	56869.25	56879.52	56881.24
22	56899.93	56910.86	56913.25
24	56933.00		56947.64
26	56968.30	56979.52	56983.84
28	57005.56	57019.85	57020.98
30	57044.63	57057.00	57065.33
32	57085.21	57098.79	

v' = 17

N	$T_1(N)$	$T_2(N)$	$T_3(N)$
0	56843.52		
2	56846.03	56854.55	56853.27
4	56850.79	56859.40	56857.82
6	56858.03	56866.94	56865.35
8	56867.85	56877.16	56875.96
10	56880.32	56890.19	56889.35
12	56895.10	56905.48	56905.45
14	56912.42	56923.45	56924.09
16	56932.13	56943.54	56945.17
18	56954.09	56965.59	56968.95
20	56978.26	56988.72	56992.29
22	57004.33	57020.25	57023.12
24	57032.45	57048.69	57051.91
26	57062.25	57078.95	

fragmentary. The assignments of Brix and Herzberg[7] for $v' > 17$ are shown in our Figs. 17 and 18. Corresponding to all of their assigned or partially assigned lines, we have measured lines almost always within 0.1 cm^{-1} of their measured lines. In addition, they have measured many, and we more, unassigned lines in the region near the dissociation limit, where we find also essentially the same discrete lines at 77 and 615 K[21]; such lines must belong to $(v',0)$ bands and have relatively low N values ($N'' \lesssim 15$), and the implication is that the upper state levels with $N' \gtrsim 14$ lie in the continuum. At high v' values approaching 19, the triplet splittings increase rapidly, and the coupling in the B state may approach Hund–Mulliken case c.[33] For $v' > 19$, the F_1 levels have not been assigned, perhaps as a result of perturbative interaction with another state dissociating to O ^3P + O ^1D. It is unclear at present how the F_1, F_2, and F_3 terms, which belong to O_u^+, 1_u, and 1_u, respectively, in case c are correlated with the dissociation limits O $^3P_{2,1,0}$ + O ^1D.

3.2.5. Satellite and Forbidden Branches

Satellite and forbidden lines, which are weak and become rapidly weaker with increasing rotational quantum number,[33] are observed only in the crowded bandhead regions. In Table 4, the wave numbers of satellite and forbidden lines with $N = 1$–9, calculated for the bands (9,0)–(17,0) from B state term values (Sec. 3.2.6), derived from the principal branch lines and the known X state term values[9] are given. Our measured values, when available, are given immediately beneath the appropriate calculated values.

3.2.6. Term Values of the B $^3\Sigma_u^-$ ($v' = 9$–17) State

The term values for the B state given in Table 5 are calculated from the accurate known term values of the X $^3\Sigma_g^-$ ($v'' = 0$) ground state[9] and the measured wave numbers of the B(v')–X(0) principal branch lines in Tables 1.9–1.17. The determination of the band origins, rotational constants, and spin splitting constants is in progress.[21]

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