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Oscillator Strengths for Transitions between $2p^33p$ and $2p^33s$ in Oxygen I, Including Configuration Interaction*

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Oscillator strengths are calculated for transitions between the various terms of $2p^33p$ and $2p^33s$ of oxygen I. Term energies for the two configurations are calculated with the inclusion of the $L(L+1)$ correction of Trees and with configuration interaction. The configurations included with $2p^33s$ are $2p^34s$ and $2s2p^5$ while $2p^34p$ is included with $2p^33p$. It is shown that the $L(L+1)$ correction should be assigned to the parent ion. Configuration interaction is included in the calculation of σ^2 as well as in the energies. The radial wave functions used in the calculation of σ^2 are Hartree wave functions without exchange.

INTRODUCTION

It has been pointed out by Condon and Shortley[1] that one should expect configuration interaction to play a significant role in the determination of the energy levels for oxygen I since the terms of the series based on different parent terms of the ground state of oxygen II lie close together. For this reason, if one is to calculate oscillator strengths for transitions between excited states of O I, the wave functions for the various states should be linear combinations of the wave functions for the separate configurations. The proper linear combination will be that obtained by the unitary transformation which will diagonalize the energy matrix. In this work, oscillator strengths for transitions between the odd-parity levels predominantly of the $2p^33s$ configuration and the even levels, for which $2p^33p$ is the most important configuration, have been calculated.

OSCILLATOR STRENGTHS

The oscillator strength, f, for a transition between the levels γSLJ and $\gamma' S'L'J'$, defined in TAS 9^4, may be written in the form

$$f(\gamma SLJ,\gamma' S'L'J') = \frac{\nu(\gamma SLJ,\gamma' S'L'J')S(\gamma SLJ,\gamma' S'L'J')}{3R(2J+1)a_0^2e^2}, \tag{1}$$

where $\nu(\gamma SLJ,\gamma' S'L'J')$ is the wave number difference between the two levels, R is the Rydberg constant expressed in wave numbers, a_0 is the radius of the first Bohr orbit, $2J+1$ is a weighting factor for the initial level, and $S(\gamma SLJ,\gamma' S'L'J')$ is a parameter called the line strength for the transition between the two levels. The line strength for a line is the sum of the strengths of the components of the line:

$$S(\gamma SLJ,\gamma' S'L'J') = \sum_M \sum_{M'} s(\gamma SLJM,\gamma' S'L'J'M'), \quad M'=M,\quad M\pm 1. \tag{2}$$

For electric dipole radiation, the line strength of the component of a line is the square of the matrix element of the electric dipole moment connecting the two states involved in the transition.

$$s(\gamma SLJM,\gamma' S'L'J'M') = \left|\int \Psi(\gamma SLJM)\mathbf{P}\Psi(\gamma' S'L'J'M')d\tau\right|^2. \tag{3}$$

Line strengths may also be written in the form[2]

$$S = S_1(L)S_2(M)\sigma^2, \tag{4}$$

where $S_1(L)$ is a factor which depends on the particular line of a multiplet and $S_2(M)$ depends on the particular multiplet of the transition array under consideration. The quantity σ is the integral $[a_0e/(4l^2-1)^{\frac{1}{2}}] \times \int R_{nl}(\rho)\rho R_{n,l-1}(\rho)d\rho$, where $R(\rho)/\rho$ is the radial wave function of the jumping electron in atomic units. $S_1(L)$ may be obtained from tables given either by White and Eliason[3] or by Russell,[4] while tables for $S_2(M)$ are given by Goldberg.[5,6]

It has been pointed out by Chandrasekhar[7] and others[8,9] that, where $R(\rho)$ is a solution of the Schrödinger equation, the dipole moment, dipole velocity, and dipole acceleration forms for the oscillator strength are equivalent. When, however, the wave functions are chosen on the basis of a variational calculation for the energy, these wave functions are most exact at moderate radial distances. This leads to a preference for the dipole velocity form. Since the radial wave functions used in these calculations were obtained by the Hartree method,[10] the integrals which were actually calculated were the dipole velocity integrals.

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[1] E. U. Condon and G. H. Shortley, *Theory of Atomic Spectra* (Cambridge University Press, Cambridge, 1935) (This shall hereafter be referred to as TAS) 2^8.

[2] D. R. Bates and A. Damgaard, Trans. Roy. Soc. (London) **A242**, 101 (1949).

[3] H. E. White and A. Y. Eliason, Phys. Rev. **44**, 753 (1933).

[4] H. N. Russell, Astrophys. J. **83**, 129 (1936).

[5] L. Goldberg, Astrophys. J. **82**, 1 (1935).

[6] L. Goldberg, Astrophys. J. **84**, 11 (1936).

[7] S. Chandrasekhar, Astrophys. J. **102**, 223 (1945).

[8] L. C. Green and N. E. Weber, Astrophys. J. 111, 582 (1950).

[9] M. N. Lewis, National Bureau of Standards Report No. 2457, 1953 (unpublished).

[10] D. R. Hartree, Proc. Cambridge Phil. Soc. **24**, 89 (1928).

$$\int_0^\infty R_{n,\,l}(\rho)\rho R_{n,\,l-1}(\rho)d\rho$$
$$=\frac{2}{\Delta\epsilon}\int_0^\infty R_{n,\,l-1}(\rho)\left[\frac{l}{\rho}R_{n,\,l}(\rho)+\frac{dR_{n,\,l}(\rho)}{d\rho}\right]d\rho. \quad (5)$$

When the initial and final states can be assigned uniquely to single configurations, σ^2 will be common to all transitions between the configurations. When, however, this unique assignment is impossible, σ^2 will depend on the pair of terms which are involved in the transition. The wave functions for the various states will be linear combinations of the individual configuration wave functions.

$$\Psi(\gamma SLJM)=a_1\Psi_1(\gamma_1 SLJM)+a_2\Psi_2(\gamma_2 SLJM)+\cdots. \quad (6)$$

The formula for the line strength will then be of the form

$$s(\gamma SLJM,\gamma' S'L'J'M')$$
$$=\left|\int \sum_i \sum_{i'} a_i a_{i'} \psi_i(\gamma_i SLJM) \times \mathbf{P}\psi_{i'}(\gamma' SL'J'M')d\tau\right|^2. \quad (7)$$

The dependence of each of the integrals on L, J, M, L', J', and M' will be the same as it would have been if the states were uniquely assigned to configurations. $S_1(L)$ and $S_2(M)$ will, therefore, be the same for each integral but the σ^2 will be different and will be of the form

$$\sigma^2=(\sum_i \sum_{i'} a_i a_{i'} I_{ii'})^2. \quad (8)$$

In order to determine the proper linear combination of configuration wave functions, the matrices for electrostatic interaction were calculated, including the off-diagonal elements connecting the different configurations. In the case of the p^3p matrix, there are, in addition, off-diagonal elements connecting terms in the same configuration, having the same term designation, but built on different terms in the parent ion. These matrices were diagonalized, and the radial integral parameters were adjusted to give the best fit between theoretical and experimental[11] term values. When this had been done, the unitary transformation matrix which would perform the diagonalization was determined. This unitary matrix determines the proper linear combination of configuration wave functions.

In the next two sections, the procedures used to diagonalize the two energy matrices will be discussed in some detail.

ODD-PARITY CONFIGURATIONS

TABLE I. Matrix elements of odd-parity configurations.

Term	Diagonal elements		Off-diagonal elements
$({}^4S)ns\ {}^5S$	$E_0(ns)-15F_2-3G_1(ns)$		R_0-3R_1
$({}^4S)ns\ {}^3S$	$E_0(ns)-15F_2+G_1(ns)$		R_0+R_1
$({}^2D)ns\ {}^3D$	$E_0(ns)-6F_2-2G_1(ns)$		R_0-2R_1
$({}^2D)ns\ {}^1D$	$E_0(ns)-6F_2$		R_0
$({}^2P)ns\ {}^3P$	$E_0(ns)$	$-2G_1(ns)$	R_0-2R_1
$({}^2P)ns\ {}^1P$	$E_0(ns)$		R_0
$2s2p^5\ {}^3P$	$E_0(sp^5)$	$-2G_1(sp^5)$	$\sqrt{2}R_1'$; $\sqrt{2}R_1''$
$2s2p^5\ {}^1P$	$E_0(sp^5)$		$\sqrt{2}R_1'$; $\sqrt{2}R_1''$

$E_0(ns)=3F_0(2p,2p)+3F_0(2p,ns)+$integrals over closed shells,
$E_0(sp^5)=10F_0(2p,2p)+5F_2(2p,2s)-20F_2(2p,2p)-G_1(2p,2s)$ +integrals over closed shells,
$R_0=3R_0(2p3s,2p4s)+$integrals over closed shells,
$F_2=F_2(2p,2p)$, $R_1=R_1(2p3s,4s2p)$,
$G_1(ns)=G_1(2p,ns)$, $R_1'=R_1(2s3s,2p2p)$,
$G_1(sp^5)=G_1(2p,2s)$, $R_1''=R_1(2s4s,2p2p)$.

The configurations that are most likely to interact with the $2p^33s$ configuration are those with terms which lie nearest to the terms of $2p^33s$. The configurations included here are $2p^34s$ and $2s2p^5$. The diagonal matrix elements for a p^3s configuration are given in TAS 5[7] in terms of three parameters, E_0, F_2, and G_1. They were checked and it was found that they were all correct, except that for ${}^3S$ the coefficient of G_1 should be $+1$ instead of -1. This correction agrees with the relations as given by Johnson[12] and by Edlén.[13] The $2s2p^5$ configuration has but two terms and two parameters, E_0 and G_1. The off-diagonal elements of the matrix contain four additional parameters. The matrix elements are given in Table I. There are, therefore, in all twelve different parameters which can be adjusted in order to fit the experimental term values. F_2 involves only $2p$ electrons, which are assumed to remain unchanged, and this parameter was considered to be the same for both configurations $2p^33s$ and $2p^34s$. Of the fourteen possible term values eleven are known experimentally.[11] The other three were determined by extrapolation of the O I isoelectronic sequence.

The parameters were evaluated in a step-by-step process. First, a least-squares calculation was made using the diagonal sums of the submatrices. This calculation gave values for $E_0(sp^5)$, $G_1(sp^5)$ and F_2 and the sums $E_0(3s)+E_0(4s)$ and $G_1(3s)+G_1(4s)$. Next, a least-squares calculation was performed using the four two by two submatrices to determine $E_0(3s)$, $E_0(4s)$, $G_1(3s)$, $G_1(4s)$, R_0, and R_1. Lastly, a least-squares calculation was made with the two three by three submatrices to determine R_1' and R_1''. The results of these calculations are given in Table II, column *b*. The fit for the ${}^3P$ and ${}^1P$ terms is not at all satisfactory. Several other procedures were tried, but none gave satisfactory results although it was possible to reduce

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[11] C. E. Moore, National Bureau of Standards Circular No. 467, 1949 (This is in book form under the title *Atomic Energy Levels.*)

[12] M. H. Johnson, Phys. Rev. **39**, 197 (1931).

[13] B. Edlén, Kgl. Svenska Vetenskapsakad. Handl. (3) **20**, No. 10 (1943).

TABLE II. Term values of $2p^3 3s$, $2p^3 4s$, and $2s2p^5$, in kaysers. (1 K = 1 cm^{-1}.)

Term	*a* Observed value, K	*b* Calculated value, K	Diff	*c* Calculated value, K	Diff
$(3s)^5S$	73 768	73 766	−2	73 702	−66
$(4s)^5S$	95 476	95 433	+33	95 444	−32
$(3s)^3S$	76 795	76 544	−251	76 798	+3
$(4s)^3S$	96 226	96 513	+287	96 324	+98
$(3s)^3D$	101 143	101 130	−13	101 168	+25
$(4s)^3D$	[122 250]	122 335	+85	122 282	+32
$(3s)^1D$	102 662	102 511	−151	102 718	+56
$(4s)^1D$	122 799	122 878	+79	122 720	−79
$(3s)^3P$	113 916	110 677	−3239	113 715	−201
$(4s)^3P$	[135 733]	140 327	+4590	135 858	+125
$(sp^5)^3P$	126 304	124 952	−1352	126 380	+76
$(3s)^1P$	115 918	119 470	+3552	115 859	−59
$(4s)^1P$	[136 083]	140 515	+4432	135 904	−179
$(sp^5)^1P$	[189 837]	181 855	−7982	190 077	+240
		$(D^2/N)^{\frac{1}{2}}=$	3042	$(D^2/N)^{\frac{1}{2}}=$	105

Values of parameters used:

$E_0(3s)$	120 385 K	114 880 K
$E_0(4s)$	140 534	134 798
$E_0(sp^5)$	180 921	189 902
F_2	2961	2585
$G_1(3s)$	730	796
$G_1(4s)$	232	198
$G_1(sp^5)$	31 982	31 949
R_0	−1485	917
R_1	−626	499
R_1'	5075	2061
R_1''	−1286	1249
α	···	565

the standard deviation to 1463 K. This particular procedure is described, and the term values obtained with it are reported, so that they may be compared with the term values obtained by a modification of this procedure which is discussed in the next paragraph.

In order to improve the fit, the $L(L+1)$ correction of Trees[14] was included in the diagonal elements of the $2p^3 3s$ and $2p^3 4s$ configurations with α taken to be the same for both configurations. This correction was not included in the diagonal terms of $2s2p^5$ since any such correction could be absorbed in the value of $E_0(sp^5)$. The same procedure was followed as that described above, and the value of α was determined by least squares using the diagonal sums. The results of this calculation are given in column *c* of Table II. The agreement between calculated and experimental values is all that can be expected in view of the extrapolation required for some of the experimental values. The extrapolated values are enclosed in brackets in column *a* of Table II. The fit might possibly be improved slightly by the inclusion of the three-by-three matrices in the determination of the parameters which effect the separation of the terms of the submatrices, but because of the other sources of error present this does not seem to be justified.

EVEN-PARITY CONFIGURATIONS

The only configuration which was included in the interaction with the $2p^3 3p$ configuration was the one with terms lying directly above it, $2p^3 4p$. There are, for these configurations, off-diagonal elements connecting terms having the same term designation in the same configuration but based on different terms of the parent ion, in addition to the off-diagonal elements connecting terms in different configurations.

The wave functions for the p^3p configurations were determined in the same manner as were the p^3s wave functions, by the application of the vector coupling formulas given in TAS 6[8]. With these wave functions, the matrix elements for electrostatic interaction were calculated, and the results, given in Table III, were compared with the matrix elements determined by Yamanouchi.[15] They are in accord except for the sign of the coefficient of G_2 in the matrix element connecting $(^2D)^3P$ with $(^2P)^3P$ and the signs of four of the off-diagonal elements connecting terms with different parentage. Yamanouchi obtained these off-diagonal elements by the method of spectroscopic stability, and the relative phases of his wave functions cannot be determined. In this paper, the relative phases of the wave functions for the terms of the parent ion were made to agree with Racah.[16]

A preliminary calculation was made on the $2p^3 3p$ configuration, ignoring the off-diagonal matrix elements, in order to obtain approximate magnitudes of the

TABLE III. Matrix elements of even-parity configurations.

Term	Diagonal elements[a]	Off-diagonal elements, different configurations, same parentage
$(^2D)^3F$	$E_0-6F_2-G_0-4G_2$	$R_0-R_0'-4R_2'$
$(^2D)^1F$	$E_0-6F_2-G_0+2G_2$	$R_0-R_0'+2R_2'$
$(^2D)^3D$	$E_0-6F_2-G_0-(17/2)G_2$	$R_0-R_0'-(17/2)R_2'$
$(^2P)^3D$	$E_0-G_0-(11/2)G_2$	$R_0-R_0'-(11/2)R_2'$
$(^2D)^1D$	$E_0-6F_2+2G_0+\frac{1}{2}G_2$	$R_0+2R_0'+\frac{1}{2}R_2'$
$(^2P)^1D$	$E_0+(3/2)G_2$	$R_0+(3/2)R_2'$
$(^4S)^5P$	$E_0-15F_2-G_0-10G_2$	$R_0-R_0'-10R_2'$
$(^4S)^3P$	$E_0-15F_2+(1/3)G_0+(10/3)G_2$	$R_0+(1/3)R_0'+(10/3)R_2'$
$(^2D)^3P$	$E_0-6F_2+(2/3)G_0-(59/6)G_2$	$R_0+(2/3)R_0'-(59/6)R_2'$
$(^2P)^3P$	$E_0-(15/2)G_2$	$R_0-(15/2)R_2'$
$(^2D)^1P$	$E_0-6F_2-G_0-(11/2)G_2$	$R_0-R_0'-(11/2)R_2'$
$(^2P)^1P$	$E_0-G_0-(5/2)G_2$	$R_0-R_0'-(5/2)R_2'$
$(^2P)^3S$	$E_0-G_0-10G_2$	$R_0-R_0'-10R_2'$
$(^2P)^1S$	E_0+3G_0	R_0+3R_0'

Connected terms	Off-diagonal elements, same configuration, different parentage	Off-diagonal elements, different configurations, different parentage
$(^2D)^3D-(^2P)^3D$	$\frac{3}{2}\sqrt{3}(-2F_2'+G_2)$	$\frac{3}{2}\sqrt{3}(-2R_2+R_2')$
$(^2D)^1D-(^2P)^1D$	$\sqrt{3}[-3F_2'+G_0-(7/2)G_2]$	$\sqrt{3}[-3R_2+R_0'-(7/2)R_2']$
$(^2D)^3P-(^2P)^3P$	$(\frac{1}{3}\sqrt{15})(9F_2'-G_0+\frac{1}{2}G_2)$	$(\frac{1}{3}\sqrt{15})(9R_2-R_0'+\frac{1}{2}R_2')$
$(^2D)^3P-(^4S)^3P$	$-(\frac{2}{3}\sqrt{5})(G_0+G_2)$	$-(\frac{2}{3}\sqrt{5})(R_0'+R_2')$
$(^2P)^3P-(^4S)^3P$	$\frac{3}{2}\sqrt{3}(G_0-5G_2)$	$\frac{3}{2}\sqrt{3}(R_0'-5R_2')$
$(^2D)^1P-(^2P)^1P$	$(\frac{3}{2}\sqrt{15})(2F_2'-G_2)$	$(\frac{3}{2}\sqrt{15})(2R_2-R_2')$

$E_0=3F_0(2p,2p)+3F_0(2p,np)$ +integrals over closed shells,

$R_0=3R_0(2p3p,2p4p)$ +integrals over closed shells,

$F_2=F_2(2p,2p)$ $\quad R_0'=R_0(2p3p,4p2p)$,

$F_2'=F_2(2p,np)$ $\quad R_2=R_2(2p3p,2p4p)$,

$G_0=G_0(2p,np)$ $\quad R_2'=R_2(2p3p,4p2p)$,

$G_2=G_2(2p,np)$.

[a] Diagonal elements of the two configurations have the same form and are obtained by replacing either $3p$, or $4p$ for np in the parameters.

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[14] R. E. Trees, Phys. Rev. **84**, 1089 (1951).

[15] T. Yamanouchi, Proc. Phys.-Math. Soc. Japan **20**, 547 (1938).

[16] G. Racah, Phys. Rev. **63**, 367 (1943).

parameters G_0 and G_2. The $L(L+1)$ correction of Trees was included with the L value from the terms in p^3p. The value of F_2 was taken to be the same as for the $2p^3ns$ configurations. When a least squares calculation was made to determine the values of E_0, G_0, G_2, and α, it was discovered that the terms grouped themselves in such a way that the terms having the same parentage had approximately the same error. Other instances where the errors in the calculated term values are a function of the L value of the parent term have been reported by Racah.[17] If the errors in the terms built on the (^4S) parent are minimized by adjusting E_0, the errors in the other terms were approximately equal to the $L(L+1)$ correction to the $2p^3ns$ configurations for terms with the same parents. This suggested that the $L(L+1)$ correction, in all the configurations of the form al^nbl', was that of the parent ion.

To check this suggestion, the values of F_2 and α were calculated for the ground state of O II. This could be done exactly since there are three terms and three parameters. This calculation gave $F_2=2627$ K and $\alpha=531$ K. These values are in reasonable agreement with $F_2=2585$ K and $\alpha=565$ K found by least squares on the odd-parity configurations.

In addition Greyber[18] has shown that, if an interaction of the form $\sum_{a,b}\mathbf{l}_a\cdot\mathbf{l}_b$ is considered, for configurations of the form al^nbl' (which is the form considered here) the predominant part of the interaction energy will be proportional to $L(L+1)$ for the L of the parent term. In the configurations under consideration, therefore, the $L(L+1)$ correction is assigned to the parent ion. (This is equivalent to building the term values on the experimental values of the parent ion.)

TABLE IV. Term values (in K) of even-parity configurations.

Term	Observed	$2p^33p$ Calculated	Diff	Observed	$2p^34p$ Calculated	Diff
$(^4S)^5P$	86 629	86 393	−236	99 094	99 389	+295
$(^4S)^3P$	88 631	89 148	+517	99 680	102 810	+3130
$(^2D)^3D$	113 295	113 158	−137	125 780	125 932	+152
$(^2D)^3F$	113 719	113 698	−21		126 522	
$(^2D)^3P$		117 158			134 072	
$(^2D)^1P$		113 307			125 707	
$(^2D)^1F$	113 995	114 206	+211		127 042	
$(^2D)^1D$	116 630	117 294	+664		136 993	
$(^2P)^3S$		126 298			139 294	
$(^2P)^3D$	127 286	127 048	−238		139 672	
$(^2P)^3P$		127 811			145 782	
$(^2P)^1P$	127 667	127 940	+273		139 983	
$(^2P)^1D$	128 595	128 161	−434		149 991	
$(^2P)^1S$	130 943	130 886	−57		160 202	

Values of the parameters used, in K:

$E_0(3p)=131\,233$ $F_2'(3p)=258,$
$E_0(4p)=139\,883$ $F_2'(4p)=81,$
$G_0(3p)=4233$ $R_0=5950,$
$G_0(4p)=1671$ $R_0'=2900,$
$G_2(3p)=143$ $R_2=80,$
$G_2(4p)=45$ $R_2'=108,$
$F_2=2585$ $\alpha=565.$

TABLE V. Calculated values of σ^2.

Transition	Wave number of line	a σ^2 Conf. int.	b σ^2 Bates and Damgaard
$(^4S)3p\ ^5P-(^4S)3s\ ^5S$	12 861	9.85	7.86
$(^4S)3p\ ^3P-(^4S)3s\ ^3S$	11 836	10.75	9.53
$(^2D)3p\ ^3F-(^2D)3s\ ^3D$	12 576	10.20	8.80
$(^2D)3p\ ^3D-(^2D)3s\ ^3D$	12 152	10.38	8.62
$(^2D)3p\ ^3P-(^2D)3s\ ^3D$	[15 990]	5.98	
$(^2D)3p\ ^1F-(^2D)3s\ ^1D$	11 333	11.49	8.30
$(^2D)3p\ ^1D-(^2D)3s\ ^1D$	13 968	7.44	7.89
$(^2D)3p\ ^1P-(^2D)3s\ ^1D$	[10 589]	11.61	
$(^2P)3p\ ^3D-(^2P)3s\ ^3P$	13 370	7.31	7.63
$(^2P)3p\ ^3P-(^2P)3s\ ^3P$	[14 096]	6.76	
$(^2P)3p\ ^3S-(^2P)3s\ ^3P$	[12 583]	9.37	
$(^2P)3p\ ^1D-(^2P)3s\ ^1P$	12 677	9.57	8.41
$(^2P)3p\ ^1P-(^2P)3s\ ^1P$	11 749	8.24	8.48
$(^2P)3p\ ^1S-(^2P)3s\ ^1P$	15 025	6.28	7.64

In order to determine the radial integral parameters with configuration interaction included, some other procedure than the one applied in the case of the odd-parity configurations was necessary. This is so since there are only thirteen experimentally known term values, and there are in all twelve parameters to be determined, while the diagonal sum of but a single submatrix is known. To employ a least-squares calculation to determine all the parameters would be unsatisfactory. In a least-squares calculation no distinction is made between large and small parameters and in order to get the best possible agreement with experiment the calculation may give unreasonable magnitudes to some of the smaller parameters.

In order to calculate some of the parameters approximately, without resort to least squares, all those which consist of only one radial integral were calculated using the same radial wave functions employed in the calculation of the σ^2 for the oscillator strengths. This left $E_0(3p)$, $E_0(4p)$, and R_0 to be determined. They were determined by a least-squares calculation on all the two-by-two submatrices. This calculation resulted in values of $E_0(3p)$ and $E_0(4p)$ which made the diagonal element for $(4p)^1S$ slightly smaller than that for $(3p)^1S$. Some arbitrary adjustments were made in the larger parameters, therefore, in order to put these matrix elements in their proper order. This adjustment actually resulted in a better fit for all of the calculated term values. The term values obtained from the final calculations are given in Table IV.

Except for the values for the ^3P terms, the calculated energies are in reasonable agreement with the experimental values. The reason that the $(^4S)^3P$ terms do not agree with experiment seems to be that, with comparatively large off-diagonal elements (∼6000 K to ∼2000 K), configuration interaction with $2p^35p$ and $2p^36p$ would be important. The term $(^4S)5p\ ^3P$ lies at 103 869 K and $(^4S)6p\ ^3P$ lies at 105 911 K, about 4000 K and 6000 K respectively above the experimental value of the $(^4S)4p\ ^3P$ term. Interaction with these configurations would lower the calculated term

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[17] G. Racah, Phys. Rev. **62**, 438 (1942).

[18] H. Greyber, Ph.D. thesis, University of Pennsylvania, 1953 (unpublished).

TABLE VI. Absorption oscillator strengths $2p^33s-2p^33p$.

Parent	$2p^33s$ level	$2p^33p$ level	f
(^2D)	$^3D_3$	$^3F_4$	0.448
	$^3D_3$	$^3F_3$	0.038
	$^3D_3$	$^3F_2$	0.001
	$^3D_2$	$^3F_3$	0.433
	$^3D_2$	$^3F_2$	0.048
	$^3D_1$	$^3F_2$	0.488
(^2D)	$^3D_3$	$^3D_3$	0.302
	$^3D_3$	$^3D_2$	0.038
	$^3D_2$	$^3D_3$	0.053
	$^3D_2$	$^3D_2$	0.237
	$^3D_2$	$^3D_1$	0.051
	$^3D_1$	$^3D_2$	0.085
	$^3D_1$	$^3D_1$	0.255
(^2D)	$^3D_3$	$^3P_2$	0.157
	$^3D_2$	$^3P_2$	0.039
	$^3D_2$	$^3P_1$	0.118
	$^3D_1$	$^3P_2$	0.003
	$^3D_1$	$^3P_1$	0.065
	$^3D_1$	$^3P_0$	0.087
(^2D)	$^1D_2$	$^1F_3$	0.470
(^2D)	$^1D_2$	$^1D_2$	0.296
(^2D)	$^1D_2$	$^1P_1$	0.202
(^2P)	$^3P_2$	$^3D_3$	0.219
	$^3P_2$	$^3D_2$	0.039
	$^3P_2$	$^3D_1$	0.003
	$^3P_1$	$^3D_2$	0.196
	$^3P_1$	$^3D_1$	0.065
	$^3P_0$	$^3D_1$	0.261
(^2P)	$^3P_2$	$^3P_2$	0.262
	$^3P_2$	$^3P_1$	0.087
	$^3P_1$	$^3P_2$	0.145
	$^3P_1$	$^3P_1$	0.087
	$^3P_1$	$^3P_0$	0.116
	$^3P_0$	$^3P_1$	0.349
(^2P)	$^3P_2$	$^3S_1$	0.107
	$^3P_1$	$^3S_1$	0.107
	$^3P_0$	$^3S_1$	0.107
(^2P)	$^1P_1$	$^1D_2$	0.537
(^2P)	$^1P_1$	$^1P_1$	0.272
(^2P)	$^1P_1$	$^1S_0$	0.086
(^4S)	$^5S_2$	$^5P_3$	0.479
	$^5S_2$	$^5P_2$	0.342
	$^5S_2$	$^5P_1$	0.205
(^4S)	$^3S_1$	$^3P_2$	0.605
	$^3S_1$	$^3P_1$	0.363
	$^3S_1$	$^3P_0$	0.121

values and would have the greater effect on the $(^4S)4p\ ^3P$ term which has the larger error.

It should be pointed out that for configuration interaction between configurations of the form al^nbl' the coefficients of the parameters in the off-diagonal elements are the same as those of corresponding parameters in the diagonal elements. Because of this, large diagonal elements will be associated with large off-diagonal elements. The resulting term values will be insensitive to changes in the parameters in the off-diagonal elements, since such changes can be approximately compensated by changes in the corresponding diagonal elements. This compensation will occur in each of the submatrices. As an example, where the coefficient of G_0 is positive that of R_0' will also be positive. As a result, making R_0' smaller and simultaneously making G_0 for the lower configuration larger and G_0 for the higher configuration smaller may result in little change in the term values. To see the effect of this, one can compare the values of G_0 and G_2 obtained by ignoring off-diagonal elements with those where G_0 and G_2 are first approximated by radial integrations and configuration interaction is included. Several investigators have determined these parameters without taking into account off-diagonal elements. Edlén[13] obtained $G_0=839$ K and $G_2=67$ K; Yamanouchi[15] did not give values for O I but they may be approximated to be $G_0\sim 1000$ K and $G_2\sim 50$ K by interpolation in the graphs in his paper. The preliminary calculations for this work gave $G_0=990$ K and $G_2=46$ K. In the final calculations including configuration interaction the values $G_0=4233$ K and $G_2=143$ K were used.

RESULTS

When the term values have been determined it is a straightforward calculation to determine the transformation matrices which will diagonalize the individual submatrices and thus determine the a_1's and a_2's of Eq. (6). When this had been done, the various values of σ^2 were calculated from Eq. (8). It was necessary to evaluate only the four integrals between the two sets of configurations $2p^3ns$ and $2p^3np$[19] since the integrals between $2p^3np$ and $2s2p^5$ will vanish. The values for σ^2 thus calculated are given in column *a* of Table V. In column *b* of Table V are given values of σ^2 calculated by the method of Bates and Damgaard[2] which uses hydrogenic wave functions and effective quantum numbers determined from experimental energies. The values for the wave numbers given in Table V are the differences between the centers of gravity of the experimental term values where these are known. If the line has not been identified, the values given (enclosed in brackets) are the differences between the calculated term values. Table VI gives the absorption oscillator strengths calculated by Eqs. (3) and (1).

Except for the transitions arising from ^3P levels, the values of σ^2 are as accurate as one might expect using the one-electron approximation and Hartree radial wave functions without exchange. The Hartree wave functions were determined by a self-consistent field calculation for the $2p^33s$ configuration. The wave functions for $3p$, $4s$, and $4p$ electrons were calculated assuming the wave functions of the core electrons to be the same as for $2p^33s$.

The results of the calculations could be improved if more energy levels were known for $2p^34p$ and if higher even-parity configurations were included in the calculations. This latter is not possible at present since only one term value is known for each of the next two configurations.

In conclusion, the author wishes to express his appreciation to Professor C. W. Ufford for suggesting this problem and for the valuable and patient assistance which he has given the author throughout the calculations. He also wishes to express his thanks to Professor L. C. Green for the help received during several informative discussions.

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[19] The calculated values of the dipole velocity integrals are -5.812 for $3s-3p$, -0.504 for $3s-4p$, 5.547 for $4s-3p$, and -12.395 for $4s-4p$. As a check on the wave functions, the dipole moment integral was calculated for $3s-3p$. It was -5.818.