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COMPARISON OF CALCULATED OSCILLATOR STRENGTHS FOR Si III*

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Abstract—Oscillator strengths have been calculated for many of the major transitions in Si III using both dipole length and dipole velocity matrix elements. Three approximations to the many-electron correlation problem are explored and compared: (1) the use of configuration interaction employing a semiempirical frozen core potential; (2) the use of configuration interaction employing a modified Hartree–Fock–Slater basis set; and (3) the use of the Coulomb approximation whereby a wavefunction is constructed with the correct asymptotic behavior. None of these methods as far as they have been carried out here is found to be fully satisfactory. Emphasis is placed upon the difficulty of calculating transition probabilities between high-lying energy levels which are strongly perturbed.

INTRODUCTION

EVER since it has become possible to obtain spectra of stars, there has been a strong demand for laboratory data on atomic lines in order to explain the observed spectral features. One of the most fundamental measures of a spectral line is its oscillator strength or transition probability. The physics required to set down the basic equations for the solution of this problem is well understood.[1] Calculations were carried out as early as 1927.[2,3] However, there still exists a large number of astrophysically important transitions for which not even the order of magnitude of the oscillator strength is known. The difficulty of performing reliable theoretical determinations of oscillator strength values appears to be accompanied by the similarly large difficulty of obtaining trustworthy oscillator strengths by experimental means. Indeed, there is a dearth of measurements on transitions between highly excited states or transitions in highly ionized atoms.[4]

Theoretically, the problem stems from the Coulomb interaction of all the electrons. The standard non-relativistic Hamiltonian (in atomic units, $e = \hbar = m = 1$) for the N-electron atom

$$\mathscr{H} = \sum_{i=1}^{N} (-\tfrac{1}{2}\nabla_i^2 - Z/r_i) + \sum_{i>j=1}^{N} 1/r_{ij} \tag{1}$$

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is not separable. For a zero-order approximation to the many-electron wavefunction it is customary to replace the second term of equation (1) by a central-field potential, or sum of central-field potentials

$$\sum_{i>j=1}^{N} 1/r_{ij} \Rightarrow \sum_{i=1}^{N} V(r_i), \tag{2}$$

which describes the motion of each electron i in the spherically averaged fields of the other electrons. The modified central field Hamiltonian now permits separable solutions and a principal quantum number n and angular momentum number l can be assigned to each electron.

If the Pauli exclusion principle is taken into account, the total wavefunction is given by a Slater determinant of one-electron wavefunctions, or more generally, by a set of Slater determinants satisfying the vector coupling rules for the total angular momentum and total spin. There are several ways to construct the substitute potentials V_i, the most popular being Coulomb approximation, Hartree self-consistent field, Hartree–Fock self-consistent field with exchange, Hartree–Fock–Slater (simplified Hartree–Fock) and the Thomas–Fermi statistical model.[1,5] Some of these methods are also used with scaling factors in order to match the observed energies.[6,7]

In the configuration interaction procedure the Slater determinants of the zero-order approximation are used to form a basis set for the expansion of the total many-electron wavefunction. In principle, the many-electron problem can be solved to any accuracy desired by including enough configuration wavefunctions in the basis set. In practice, the expansion must be truncated and the resulting wavefunction is merely an improved approximation to the true wavefunction, consisting of a finite linear combination of Slater determinants which diagonalize the corresponding (finite) $\mathscr{H}$-matrix.

In this paper we compare several different methods for calculating oscillator strengths for the two-electron spectrum of Si III, which is of particular astrophysical importance in hot stars.[8] Often after completing a complex and lengthy procedure to obtain many-electron wavefunctions, there is no way to determine whether that method can be trusted to provide reliable oscillator strengths. By comparing three different methods we hope to acquire a measure of confidence in the use of those oscillator strengths for which the calculations are in good agreement as well as draw attention to the existence of certain recalcitrant cases for which the oscillator strengths found by any of the methods are in poor agreement. In this way we may be able to gain insight into the nature of electronic transitions in many-electron atoms.

COMPUTATIONAL METHODS AND RESULTS

In the calculation of TREFFTZ,[9] the effect of the core electrons on the two valence electrons is approximated by a semi-empirical potential which gives the correct term values of the lowest states of Si IV. The inner of the two valence electrons is described by an eigenfunction $P(n_i l_i)$ in this semi-empirical potential. For the outer electron it is assumed that the core is shielded by the charge distribution $P^2(n_i l_i)$ of the inner electron. If we denote the eigenfunction of the outer electron by $P(n_0 l_0)$, the basis set for the configuration

interaction calculation is composed of functions of the form

$$\psi(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{\sqrt{2}}\{r_1^{-1}P(n_i l_i|r_1)r_2^{-1}P(n_0 l_0|r_2)W[l_i(1), l_0(2), L] + (-1)^{S+L-l_i-l_0}r_1^{-1}P(n_0 l_0|r_1)r_2^{-1}P(n_i l_i|r_2)W[l_0(1), l_i(2), L]\}, \quad (3)$$

where $W[l_1(1), l_2(2), L]$ is a normalized eigenfunction of the angles $\theta_1, \phi_1, \theta_2, \phi_2$, and S and L are the total spin and orbital angular momenta, respectively. Note that in using equation (3) one must be sure to take into account the non-orthonormality of the different basis set wavefunctions.

The latter complication is avoided in Zare's procedure.[10,11] He uses a modified form of the Hartree–Fock–Slater method[12] which incorporates the improvements suggested by LATTER[13] and by LINDGREN.[14] In this procedure, which is fully described elsewhere,[15] all the electrons move under the action of the same universal exchange potential. Spin-orbitals having the same set of (l_i, l_0) angular momenta are then forced to be orthogonal to one another since the radial part of each spin orbital is derived from the same radial wave equation. Since different sets of valence spin-orbitals differ by at least one angular momentum quantum number, the two-electron wavefunctions of the basis set are orthonormal.

Oscillator strengths may be calculated via the dipole length or via the dipole velocity formula. The former uses the matrix elements $\langle\psi_i|\mathbf{r}_1+\mathbf{r}_2|\psi_f\rangle$, the latter the matrix elements $\langle\psi_i|\nabla_1+\nabla_2|\psi_f\rangle$. For exact many-electron wavefunctions it may be shown that

$$|\langle\psi_i|\mathbf{r}_1+\mathbf{r}_2|\psi_f\rangle|^2 = \left(\frac{1}{E_i-E_f}\right)^2 |\langle\psi_i|\nabla_1+\nabla_2|\psi_f\rangle|^2 \quad (4)$$

where in equation (4) the energy is in atomic units. In evaluating the energy difference E_i–E_f in the above formula we have inserted the experimentally determined values with the hope that this will give a more realistic picture of the discrepancies between the dipole length and the dipole velocity results. However, we find that the major difference between oscillator strengths calculated by the two methods can be attributed to the lack of agreement between the two types of matrix elements rather than to the choice of experimental or calculated energy values, E_i–E_f, in equation (4).

We present in Appendix I the results of our various oscillator strength calculations. Under the column heading marked "gf-values" we give two entries for each transition. The upper entry is the dipole length value, and the lower entry is the dipole velocity value. Examination of Appendix I gives vivid proof of the well known but often forgotten fact that agreement between dipole length and dipole velocity calculations does *not* mean that the oscillator strength is correct. Indeed there is practically no way of independently judging the reliability of our gf-values. Clearly more extensive calculations as well as calculations by other different methods are needed, and whenever possible, more laboratory measurements must be made in order to decide which gf-values given in Appendix I are most likely to be correct.

Here a basic difficulty, first pointed out by HYLLERAAS,[16] should be mentioned. We are interested in describing the electronic correlation effects present in high-lying members of Rydberg series which are close to the ionization limit. The complete basis set should consist of a Rydberg series of bound states and a continuum. However, we have not found

it feasible to include the contribution of the continuum states to the expansion, and hence we use an incomplete basis set. Thus the inclusion of more and more bound state configurations in the expansion basis set does not guarantee that we will converge to the correct many-electron wavefunction, especially for high-lying levels.

Wavefunctions have been calculated for almost all the terms given in the latest revision of Moore's tables[17] for Si III, and we present in Table 1 a comparison of Moore's designation of the term values with those we have used in Appendix I. Our designation represents

TABLE 1. COMPARISON OF DESIGNATION AND LEADING TERMS IN THE WAVEFUNCTIONS FOR STATIONARY STATES OF Si III

Series	Designation		Leading terms	
	This paper*	Moore	Zare	Trefftz
^1S	$3s^2$	$3s^2$	$3s^2$	$3s^2$
	$3p^2$	$3p^2$	$3p^2$	$3s4s$
	$3s4s$	$3s4s$	$3s4s$	$3p^2$
$^1P^0$	$3s3p$	$3s3p$	$3s3p$	$3s3p$
	$3s4p$	$3s4p$	$3s4p$	$3s4p$
	$3s5p$*	$3s5p$	$3s5p$	$3s5p$; $3p4s$
	$3p4s$*	$3p3d$	$3s6p$; $3p4s$†	$3p4s$; $3s5p$
	$3s6p$*	$3s6p$	$3s6p$; $3p4s$†	$3s6p$
	$3p3d$*	$3p4s$	$3p3d$	$3s7p$; $3p3d$
	$3s7p$*	$3s7p$		$3s7p$; $3p3d$
^1D	$3p^2$*	$3p^2$	$3p^2$; $3s3d$	$3p^2$; $3s3d$
	$3s3d$*	$3s3d$	$3s3d$; $3p^2$	$3s3d$; $3p^2$
	$3s4d$	$3s4d$	$3s4d$	$3s4d$
$^1F^0$	$3s4f$	$3s4f$		$3s4f$
	$3s5f$	$3s5f$		$3s5f$
	$3p3d$*	$3p3d$		$3s6f$; $3p3d$
	$3s6f$*	$3s6f$		$3s6f$; $3p3d$
	$3s7f$*	$3s7f$		$3s7f$; $3p3d$
^3D	$3s6d$*	$3s6d$		$3s6d$
	$3p4p$*	$3p4p$		$3p4p$; $3s6d$
	$3s7d$*	$3s7d$		$3s7d$
$^3F^0$	$3p3d$*	$3p3d$		$3p3d$; $3s4f$
	$3s4f$*	$3s4f$		$3s4f$; $3p3d$
	$3s5f$	$3s5f$		$3s5f$

* An asterisk is used when strong mixing is suspected.

† In Zare's calculation the character of the $3p4s$ configuration is swallowed up by the other interacting configurations so that no energy level has the $3p4s$ configuration as the leading term of its wavefunction.

the leading configuration in our expansion. In previous work, ZARE[10] has introduced the concept of the *spectral purity* of a configuration interaction wavefunction. Spectral purity is defined as the square of the leading coefficient in the wavefunction expansion. In Table 1 and Appendix I a superscript asterisk is used to denote those configurations which are strongly mixed, i.e. in one or both of our calculations the spectral purity is below 80 per cent. Terms not quoted in Table 1 agree with Moore's designation and are not strongly mixed. It should be noted that when the spectral purity of a configuration drops close to or below 50 per cent, the assignment of a single configuration label is quite misleading and of doubtful significance.

The most striking discrepancy in Trefftz's and Zare's calculations appears in the ^1S series where the $3s4s$ term is interchanged with $3p^2$. The ordering of these two terms is

difficult to calculate because both the energy splitting and the ratio of the configuration interaction matrix element $(3s4s\ ^1S|\mathscr{H}|3p^2\ ^1S)$ to the energy splitting are small. A more extensive Hartree–Fock calculation with configuration interaction by WEISS[18] confirms Zare's order of terms. Accordingly, Trefftz' values for transitions involving the $3s4s$ and $3p^2\ ^1S$ terms are given in parentheses. Trefftz' ansatz of describing the unexcited electron by a wavefunction of the next higher ion as though the other electron did not exist, is not fully satisfactory for low-lying levels. On the other hand, for the highly excited levels, Zare's universal potential, which is constructed to describe optimally the low-lying levels, is not very realistic. Here Trefftz' wavefunctions may be somewhat superior.

If a perturbing state lies between highly excited states of a normal series, the different choice of zero-order configuration wavefunctions results in the maximum perturbation being displaced among the strongly interacting configurations. The weights of the interacting configuration are also redistributed among the different terms of the normal series. The $3p4s$ term in the $^1P^0$ series exemplifies this confusing situation (see Table 1).

In addition to the calculated dipole lengths and dipole velocity gf-values appearing in Appendix I we also give (in column one) the vacuum wavelengths corresponding to the energy differences between the centers of gravity of the multiplets as found in Moore's tables. In column two of Appendix I we list our designation for the transition. In the final column of Appendix I we quote Coulomb approximation values when neither of the two states of the transition are strongly mixed. Since our definition of "no strong mixing" permits a mixing coefficient as large as $\pm 0{\cdot}45$ for a single perturbing configuration, we cannot expect Coulomb approximation results to be always reliable. On the other hand, Coulomb approximation wavefunctions do have the correct asymptotic behavior for large r, which certainly is important for highly excited states. We cannot guarantee this for our wavefunctions. For the reasons given above we have omitted from Appendix I Coulomb approximation values for all transitions involving $3p^2\ ^1S$ or $3s4s\ ^1S$. Also, we do not list a value when the orbit of the "jumping" electron is clearly inside the orbit of the other electron. Some of the Coulomb approximation values refer to the higher ionization limit $3p\ ^2P^0$ of Si IV. This is noted in parentheses.

It was found that the semi-convergent series for the r-matrix elements in the Coulomb approximation method does indeed suffer from a lack of convergence. BATES and DAMGAARD[19] have suggested a cutoff which neglects all powers of r smaller than r^2 in the integral $\int P(n_1l_1|r)rP(n_2l_2|r)\,dr$. In the last column of Appendix I the first number quoted was obtained using this cutoff. The second number quoted was obtained using a cutoff at the smallest term in the expansion of $\int P(n_1l_1|r)rP(n_2l_2|r)\,dr$, the so-called "best" cutoff. Neither method gives a smooth curve for Bates–Damgaard's $\mathscr{I}$ integral when the difference between the effective principal quantum numbers is held constant. Both give the same result as calculated by BATES and DAMGAARD[19] for integer values of the effective principal quantum number belonging to the larger l value. Since the deviations from a smooth behavior of the $\mathscr{I}$ integral have a certain absolute magnitude, the relative errors may become very large near a root of the $\mathscr{I}$ function.

Attention of the reader is called to the fact that there are many citations in the literature to oscillator strengths obtained from *the* Coulomb approximation. However, our calculations show that there is not one Coulomb approximation value, but many, depending upon the choice of the cutoff used.

In general we regard the strong transitions cited in Appendix I to be more reliable than the weak ones. An exception to this is the so-called two-electron double jumps which are forbidden in the central field approximation. Since the magnitude of these transitions is extremely sensitive to the departure from a central-field description, the results are heavily influenced by what minor (in the sense of contributing to the energy) configurations have been included in the basis set. Two such cases where Zare's calculations give a strong transition while Trefftz' do not are the $3s4d\,^3D - 3p3d\,^3P^0$ transition at $\lambda \sim 6830$ Å and the $3p3d\,^3P^0 - 3s5d\,^3D$ transition at $\lambda \sim 9221$ Å. There are other cases of poor agreement in the $^3P^0 - {}^3D$ transitions even though the configuration interaction pictures presented by Trefftz and Zare are quite similar. As would be expected, the singlet transitions $^1P^0 - {}^1D$, where correlation effects are more important, show some striking discrepancies. Here Table 1 provides some explanation. The interfering term $3p4s$ lies lower in Trefftz' calculation than in Zare's. Also Trefftz took the configuration $3s7p$ into account whereas Zare neglected it. This appears to account for the apparent disagreement in the $3s3d\,^1D - 3p3d\,^1P^0$ transition at $\lambda \sim 1425$ Å.

Zare did not calculate the $^{1,3}P$ terms of even parity or the $^{1,3}D^0$ terms of odd parity. However, these terms should not be critical since there is not much configuration interaction. Parity prohibits interaction with the main series $(3s, nl)\,^{1,3}L$ $(l = L)$ terms. It remains to be seen how reliable the gf-values given in Appendix I are for transitions to the "normal" series $^{1,3}P^0$, $^{1,3}D$. Also, transitions involving the $^{1,3}F^0$ terms could not be compared. These values should be accepted with at least as much reservation as the ones of the lower L's. Again asterisks indicate heavy mixing in both series.

For some transitions the results may be improved by other methods. Wavefunctions for the lowest state of a series may be calculated by Froese's program[20] which is a configuration interaction procedure based on the Hartree–Fock energy minimum principle. By an iterative process it determines the best radial dependence of the one-electron wavefunctions together with the mixing parameters. For configuration interaction between states near the first ionization limit the Many-Channel-Quantum-Defect Theory[21] may hold promise. It deduces an interaction matrix (closely related to the reaction matrix above the ionization limit) from experimental term values. Since this process leads to several solutions to the interaction matrix, it must be complemented by auxiliary methods, such as those quoted here, to determine which solution is the correct one. The method has the advantage of giving the correct asymptotic behavior of the wavefunction for large r. Finally we must caution against the indiscriminate use of the Z-expansion method of LAYZER[22] whereby one only takes into account the configuration interaction among those configurations built up from spin-orbitals having the same principal quantum numbers (i.e. the same "complex"). For high-lying states of atoms, even for doubly ionized silicon, the different interacting configurations have failed to sort themselves out by complexes.*

* The Z-expansion method may be used if the separation of the different ionization limits of a complex is less than the separation between the energy levels of the different principal quantum numbers of the considered series. In our case the ionization limits of the Si III complexes are given by the ground state 3^2S and the exeited state 3^2P^0 of Si IV with an energy difference of 71 590 cm^{-1} = 0·6524 Ry. For all but the lowest member of the different Si III series, this energy difference is larger than the difference between neighboring energy levels of different principal quantum number.

As has been shown by the presentation of our data in Table 1 and Appendix I, correlation effects in the excited states of many-electron atoms are by no means well understood. Much remains to be done before all the transition probabilities needed can be supplied with an accuracy of, say, 20 per cent. A particularly pressing challenge is to find and demonstrate a simple means of accurately calculating oscillator strengths for transitions involving strongly perturbed high-lying excited states. We should like to add a warning for anyone who wants to use the results of Appendix I: *Caveat emptor.*

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APPENDIX I. CALCULATIONS OF OSCILLATOR STRENGTHS FOR Si III TRANSITIONS

Comparison of three different methods

λ (Å) (Vacuum)	Designation*	gf-Values		
		Trefftz	Zare	Coulomb approximation†
		^1S—$^1P^0$ Transitions		
1207	$3s^2 - 3s3p$	1·61 1·76	1·70 1·58	1·82; 1·88

λ (Å) (Vacuum)	Designation*	gf-Values Trefftz	Zare	Coulomb approximation†
		$^1S - {}^1P^0$ Transitions		
567	$3s^2 - 3s4p$	0·009 0·017	0·020 0·017	0·020 ; 0·015
466	$- 3s5p$*	0·024 0·033	0·038 0·015	
437	$- 3p4s$*	0·007 0·019	0·000 0·003	
1417	$3s3p - 3p^2$	(0·65) (0·55)	0·847 0·825	
1313	$- 3s4s$	(0·30) (0·31)	0·137 0·084	
800	$- 3s5s$	0·043 0·040	0·071 0·037	0·057 ; 0·051
678	$- 3s6s$	0·019 0·015	0·021 0·014	0·021 ; 0·018
4340	$3p^2 - 3s4p$	(0·98) (0·39)	0·084 0·157	
1637	$- 3s5p$*	(0·52) (0·56)	0·046 0·018	
1329	$- 3p4s$*	(1·00) (0·94)	0·172 0·079	
1235	$- 3s6p$*	(0·156) (0·153)	0·000 0·001	
1212	$- 3p3d$*	(0·043) (0·029)	2·14 1·81	
5741	$3s4s - 3s4p$	(0·056) (0·010)	0·740 0·614	
1803	$- 3s5p$*	(0·0081) (0·0087)	0·307 0·193	
1436	$- 3p4s$*	(0·066) (0·057)	0·876 0·395	
1328	$- 3s6p$*	(0·22) (0·14)	0·613 0·251	
1301	$- 3p3d$*	(1·29) (0·64)	0·000 0·017	
3186	$3s4p - 3s5s$	0·64 0·55	0·616 0·700	0·58 ; 0·58
1856	$- 3s6s$	0·13 0·09	0·121 0·125	0·087 ; 0·084
1514	$- 3s7s$	0·062 0·040		0·032 ; 0·030
		$^3S - {}^3P^0$ Transitions		
996	$3s3p - 3s4s$	1·11 1·00	0·987 0·963	0·73 ; 0·71
653	$- 3s5s$	0·18 0·15	0·112 0·132	0·112 ; 0·106
566	$- 3s6s$	0·062 0·051	0·036 0·043	0·041 ; 0·038

λ (Å) (Vacuum)	Designation*	gf-Values Trefftz	Zare	Coulomb approximation†
		$^3S - {}^3P^0$ Transitions		
4561	$3s4s - 3s4p$	3·51 3·41	3·54 2·80	3·71; 3·73
1623	$- 3s5p$	0·026 0·047	0·019 0·058	0·010; 0·008
1591	$- 3p3d$	0·21 0·25	0·086 0·037	
1364	$- 3p4s$	1·97 1·76	3·85 2·35	
1234	$- 3s6p$	0·0030 0·0000	0·071 0·001	0·005; 0·004
3239	$3s4p - 3s5s$	2·18 1·98	2·06 1·76	1·94; 1·92
1841	$- 3s6s$	0·29 0·25	0·269 0·221	0·27; 0·26
1496	$- 3s7s$	0·12 0·10		0·096; 0·092
6835	$3s5p - 3s6s$	2·98 2·68	1·89 1·81	2·80; 2·79
3683	$- 3s7s$	0·35 0·32		0·38; 0·37
7473	$3p3d - 3s6s$	0·13 0·14		
3860	$- 3s7s$	0·021 0·021		
		$^1P - {}^1P^0$ Transitions		
625	$3s3p - 3p4p$	0·11 0·015		0·094; 0·089 (3p)
1506	$3s4p - 3p4p$	1·79 1·18		
		$^3P - {}^3P^0$ Transitions		
1299	$3s3p - 3p^2$	4·83 4·97		4·46; 4·54 (3p)
513	$- 3p4p$	0·001 0·02		0·0003; 0·0000 (3p)
2206	$3p^2 - 3s4p$	0·0007 0·0000		
1176	$- 3s5p$	0·14 0·04		
1159	$- 3p3d$	6·53 4·44		4·00; 4·13 (3p)
1034	$- 3p4s$	0·50 0·90		1·54; 1·50 (3p)
1374	$3s4p - 3p4p$	3·16 2·38		

λ (Å) (Vacuum)	Designation*	gf-Values Trefftz	Zare	Coulomb approximation†
		$^3P - {}^3P^0$ Transitions		
3024	$3s5p - 3p4p$	0·0006 0·010		
3142	$3p3d - 3p4p$	1·98 2·15		0·51; 0·67 (3p)
4676	$3p4s - 3p4p$	2·14 2·65		3·72; 3·74 (3p)
		$^1P^0 - {}^1D$ Transitions		
2543	$3s3p - 3p^2$*	0·089 0·082	0·181 0·172	
1207	$- 3s3d$*	4·66 4·57	4·91 4·53	
823	$- 3s4d$	0·55 0·33	0·388 0·346	0·015; 0·010
691	$- 3s5d$	0·050 0·024	0·003 0·025	0·004; 0·009
634	$- 3s6d$	0·0033 0·0027	0·000 0·004	0·010; 0·011
1843	$3p^2$* $- 3s4p$	0·54 0·60	0·414 0·317	
1083	$- 3s5p$*	0·37 0·35	0·162 0·149	
939	$- 3p4s$*	0·34 0·35	0·297 0·219	
891	$- 3s6p$*	0·009 0·018	0·135 0·097	
879	$- 3p3d$*	0·10 0·024	0·000 0·017	
9326	$3s3d$* $- 3s4p$	0·48 0·014	0·479 0·109	
2051	$- 3s5p$*	0·29 0·22	0·084 0·040	
1589	$- 3p4s$*	0·66 0·43	0·241 0·073	
1457	$- 3s6p$*	0·26 0·12	0·001 0·000	
1425	$- 3p3d$*	0·33 0·09	1·27 0·881	
3591	$3s4p - 3s4d$	2·81 2·30	2·80 2·96	3·76; 3·67
1954	$- 3s5d$	0·024 0·010	0·035 0·010	0·098; 0·099
1561	$- 3s6d$	0·030 0·024	0·018 0·042	0·003; 0·0003
9803	$3s4d - 3s5p$*	1·25 0·63	1·42 0·927	

λ (Å) (Vacuum)	Designation*	gf-Values Trefftz	Zare	Coulomb approximation†
		$^1P^0 - {}^1D$ Transitions		
4104	$3s4d - 3p4s$*	0·71 0·39	0·181 0·123	
3327	$- 3s6p$*	0·23 0·16	0·355 0·303	
3163	$- 3p3d$*	0·018 0·002	0·113 0·045	
		$^3P^0 - {}^3D$ Transitions		
1112	$3s3p - 3s3d$	7·82 7·74	7·97 7·70	7·93; 8·26
673	$- 3s4d$	0·039 0·022	0·068 0·046	0·166; 0·211
574	$- 3s5d$	0·0036 0·0042	0·003 0·002	0·014; 0·027
534	$- 3s6d$*	0·024 0·016	0·007 0·021	
521	$- 3p4p$*	0·089 0·055	0·116 0·076	
3091	$3s3d - 3s4p$	2·05 2·26	2·34 1·75	2·00; 2·00
1388	$- 3s5p$	0·0032 0·0044	0·381 0·230	
1365	$- 3p3d$	2·94 1·56	2·98 1·78	
1194	$- 3p4s$	0·66 0·22	0·002 0·004	
1093	$- 3s6p$	0·087 0·060	0·102 0·049	0·028; 0·222
3802	$3s4p - 3s4d$	10·9 8·9	10·1 11·6	11·2; 10·3
1931	$- 3s5d$	0·050 0·018	0·061 0·029	0·24; 0·11
1539	$- 3s6d$*	0·17 0·20	0·235 0·310	
1436	$- 3p4p$*	3·91 3·76	5·75 3·80	
7464	$3s4d - 3s5p$	4·34 4·52	3·54 2·75	
6830	$- 3p3d$	0·082 0·078	1·40 0·76	
3988	$- 3p4s$	0·25 0·16	0·087 0·064	
3045	$- 3s6p$	0·34 0·30	0·347 0·245	0·28; 0·28
8267	$3s5p - 3s5d$	14·1 11·8	10·5 14·5	

λ (Å) (Vacuum)	Designation*	gf-Values Trefftz	Zare	Coulomb approximation†
		$^3P^0 - {}^3D$ Transitions		
3952	$3s5p - 3s6d$*	0·34	0·430	
		0·19	0·253	
3339	$- 3p4p$*	0·011	0·509	
		0·063	0·136	
9221	$3p3d - 3s5d$	0·57	3·87	
		0·39	5·47	
4157	$- 3s6d$*	0·064	0·002	
		0·025	0·025	
3484	$- 3p4p$*	0·31	0·051	
		0·25	0·005	
7343	$3p4s - 3s6d$*	0·78	1·21	
		0·44	1·32	
5474	$- 3p4p$*	5·12	4·44	
		6·22	5·64	
		$^3P - {}^3D^0$ Transitions		
1143	$3p^2 - 3p3d$	12·7		12·1 ; 12·5 ($3p$)
		10·4		
3267	$3p3d - 3p4p$	1·54		1·60 ; 2·00 ($3p$)
		2·34		
		$^1D - {}^1D^0$ Transitions		
1208	$3p^2$* $- 3p3d$	2·75		
		2·33		
2547	$3s3d$* $- 3p3d$	0·037		
		0·098		
		$^3D - {}^3D^0$ Transitions		
1342	$3s3d - 3p3d$	4·35		
		3·75		
6308	$3s4d - 3p3d$	0·006		
		0·002		
10380	$3p3d - 3s5d$	0·004		
		0·012		
4378	$- 3s6d$*	0·033		
		0·039		
3638	$- 3p4p$*	0·45		
		0·42		
3159	$- 3s7d$*	0·087		
		0·063		
		$^1D - {}^1F^0$ Transitions		
1210	$3p^2$* $- 3s4f$	2·17		
		1·95		
968	$- 3s5f$	0·89		
		0·77		
883	$- 3p3d$*	0·36		
		0·29		
822	$- 3s6f$*	0·29		
		0·054		

λ (Å) (Vacuum)	Designation*	gf-Values Trefftz	Zare	Coulomb approximation†
		$^1D - {}^1F^0$ Transitions		
2560	$3s3d^* - 3s4f$	2·15 1·01		
1673	$-3s5f$	1·00 0·94		
1436	$-3p3d^*$	2·76 2·31		
1280	$-3s6f^*$	4·25 2·13		
1182	$-3s7f^*$	3·51 3·06		
4718	$3s4d - 3s5f$	3·36 2·23		6·29; 6·54
3217	$-3p3d^*$	0·009 0·12		
2529	$-3s6f^*$	0·80 0·80		
2172	$-3s7f^*$	1·34 1·98		
		$^3D - {}^3F^0$ Transitions		
1782	$3s3d - 3p3d^*$	0·000 0·12		
1501	$-3s4f^*$	14·8 14·4		
1145	$-3s5f$	4·05 3·64		2·84; 2·91
1005	$-3s6f$	1·56 1·44		1·18; 1·23
936	$-3s7f$	0·64 0·73		0·61; 0·65
39403	$3p3d^* - 3s4d$	0·43 0·28		
3568	$-3s5d$	0·063 0·021		
2425	$-3s6d^*$	0·40 0·012		
2179	$-3p4p^*$	2·23 1·05		
12545	$3s4d - 3s4f^*$	5·24 3·53		
3488	$-3s5f$	5·87 6·24		6·69; 6·74
2450	$-3s6f$	2·04 2·12		2·22; 2·28
2076	$-3s7f$	0·77 0·96		1·02; 1·06
5709	$3s4f^* - 3s5d$	1·89 1·15		

λ (Å) (Vacuum)	Designation*	gf-Values Trefftz	Zare	Coulomb approximation†
		$^3D - {}^3F^0$ Transitions		
3255	$3s4f$*$-3s6d$*	0·57 0·18		
2827	$-3p4p$*	0·71 0·22		

* An asterisk is used when strong mixing is suspected.

† The first entry in this column is obtained with a Bates–Damgaard cutoff; the second entry was obtained with the "best" cutoff. See text.