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$1/Z$-expansion study of the $1s^2 2s^2\ {}^1S$, $1s^2 2s 2p\ {}^1P$, and $1s^2 2p^2\ {}^1S$ states of the beryllium isoelectronic sequence

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A Z-expansion procedure is used to obtain eigenvalues and eigenfunctions for the $1s^2 2s^2\ {}^1S$, $1s^2 2p^2\ {}^1S$, and $1s^2 2s 2p\ {}^1P$ states of the beryllium isoelectronic sequence. The degeneracy effects associated with the $1s^2 2s^2\ {}^1S$ and the $1s^2 2p^2\ {}^1S$ states are included to every order in the perturbative procedure. Z expansions of the dipole length and dipole velocity forms of the oscillator strength for the $1s^2 2s^2\ {}^1S$-$1s^2 2s 2p\ {}^1P$ and $1s^2 2s 2p\ {}^1P$-$1s^2 2p^2\ {}^1S$ transitions are compared with the results of calculations using individual values of the nuclear charge Z.

I. INTRODUCTION

In recent papers,[1,2] selected states of the lithium isoelectronic sequence ($1s^2 2s\ {}^2S$, $1s^2 3s\ {}^2S$, $1s^2 2p\ {}^2P$, $1s^2 3p\ {}^2P$, and $1s^2 3d\ {}^2D$) were studied using a $1/Z$-expansion method.[3] In this paper we extend the study to states of the beryllium isoelectronic sequence which are degenerate in zero order. Z expansions for the energies and eigenfunctions of the $1s^2 2s^2\ {}^1S$, $1s^2 2p^2\ {}^1S$, and $1s^2 2s 2p\ {}^1P$ states of the entire beryllium isoelectronic sequence are calculated and used to obtain Z expansions of the oscillator strengths for the $1s^2 2s^2\ {}^1S$-$1s^2 2s 2p\ {}^1P$ and the $1s^2 2s 2p\ {}^1P$-$1s^2 2p^2\ {}^1S$ transitions.

II. THEORY

The eigenfunctions and eigenvalues are solutions to the nonrelativistic Schrödinger equation

$$\left(\sum_{i=1}^{4} -\tfrac{1}{2} \vec{\nabla}_i^2 - \frac{Z}{\vec{r}_i} + \sum_{i<j}^{4} \frac{1}{\vec{r}_{ij}} \right) | \psi_n \rangle = \mathcal{E}_n | \psi_n \rangle , \tag{1}$$

where $\vec{r}_i$ is the position vector (in atomic units) of the ith electron with respect to the nucleus. The Z-expansion method is developed by choosing the unit of energy to be Z^2 a.u. and the unit of length to be Z^{-1} a.u. If H_0 is the hydrogenic Hamiltonian and V is the interelectronic repulsion term, $V = \sum_{i<j}^{4} 1/|\vec{\rho}_i - \vec{\rho}_j|$, where $\vec{\rho}_i = \vec{r}_i Z$ a.u., the Hamiltonian is given by

$$H = H_0 + (1/Z)\, V . \tag{2}$$

The eigenfunctions and eigenvalues may be expanded in the form

$$| \psi_n \rangle = \sum_{s=0}^{\infty} Z^{-s} | \psi_n^{(s)} \rangle , \tag{3}$$

$$E_n = \sum_{s=0}^{\infty} Z^{-s} E_n^{(s)} , \tag{4}$$

where

$$(H_0 - E_n^{(0)}) | \psi_n^{(0)} \rangle = 0 , \tag{5}$$

$$(H_0 - E_n^{(0)}) | \psi_n^{(s)} \rangle + (V - E_n^{(1)}) | \psi_n^{(s-1)} \rangle - \sum_{r=2}^{s} E_n^{(r)} | \psi_n^{(s-r)} \rangle = 0 . \tag{6}$$

These equations are equivalent to the variational statement $\delta J_n^{(s)} = 0$, where the function $J_n^{(s)}$ is obtained by substituting Eqs. (3) and (4) into the functional

$$E_n = \frac{\langle \psi_n | H | \psi_n \rangle}{\langle \psi_n | \psi_n \rangle} \tag{7}$$

to obtain

$$J_n^{(s)} = \langle \psi_n^{(s)} | H_0 - E_n^{(0)} | \psi_n^{(s)} \rangle + 2 \langle \psi_n^{(s)} | V - E_n^{(1)} | \psi_n^{(s-1)} \rangle - \sum_{r=2}^{2s-1} E_n^{(r)} \sum_{q=s-r}^{r} \langle \psi_n^{(q)} | \psi_n^{(2s-r-q)} \rangle . \tag{8}$$

Following Dalgarno and Drake[3] we introduce the trial form

$$| \psi_n^{(s)} \rangle = \sum_{k=1}^{N} a_k^{(s)} | \phi_k \rangle , \tag{9}$$

where one of the functions, ϕ_k, is $\psi_n^{(0)}$ and the set satisfies

$$\begin{gathered} \langle \phi_k | H_0 | \phi_{k'} \rangle = \epsilon_k \delta_{kk'}, \quad k, k' = 1, 2, \ldots, N \\ \langle \phi_k | \phi_{k'} \rangle = \delta_{kk'} . \end{gathered} \tag{10}$$

This leads to the iterative solutions

$$\langle \psi_n^{(s)} | = \sum_{k \neq n}^{N} \frac{\langle \psi_n^{(s-1)} | V | \phi_k \rangle \langle \phi_k |}{\epsilon_n - \epsilon_k} - \sum_{k \neq n}^{N} \sum_{p=1}^{s} \frac{E_n^{(p)} \langle \psi_n^{(s-p)} | \phi_k \rangle \langle \phi_k |}{\epsilon_n - \epsilon_k} , \tag{11}$$

$$E_n^{(s)}=\langle\psi_n^{(s-1)}\,|\,V\,|\,\psi_n^{(0)}\rangle-\sum_{p=1}^{s-1}E_n^{(p)}\langle\psi_n^{(s-p)}\,|\,\psi_n^{(0)}\rangle\ . \tag{12}$$

Using the Wigner $2n+1$ rule $E_n^{(2s)}$ and $E_n^{(2s+1)}$ can be expressed in terms of the eigenfunction through $\psi_n^{(s)}$:

$$E_n^{(2s)}=\langle\psi_n^{(s-1)}\,|\,V\,|\,\psi_n^{(s)}\rangle-{\sum_{r=0}^{s-1}}'{\sum_{t=0}^{s}}'E_n^{(2s-r-t)}\langle\psi_n^{(r)}\,|\,\psi_n^{(t)}\rangle\ , \tag{13}$$

$$E_n^{(2s+1)}=\langle\psi_n^{(s)}\,|\,V\,|\,\psi_n^{(s)}\rangle-{\sum_{r=0}^{s}}'{\sum_{t=0}^{s}}'E_n^{(2s+1-r-t)}\langle\psi_n^{(r)}\,|\,\psi_n^{(t)}\rangle\ , \tag{14}$$

where the primed summations mean that the term $r=t=0$ is omitted. If there is no degeneracy, these recurrence relationships can be evaluated immediately. If, however, the state under investigation is degenerate in zero order with one or more states of the same symmetry, this degeneracy must be resolved and Eqs. (11)–(14) modified to account for the degeneracy at each step in the iterative scheme. We assume an n-fold degeneracy lifted in first order, as occurs in the beryllium sequence for the $1s^2 2s^2\ {}^1S$ and the $1s^2 2p^2\ {}^1S$ states. The general case of an n-fold degeneracy lifted in nth order is treated by Hirschfelder and Certain.[4]

Without loss of generality we may assume that the n degenerate states of H_0 are ϕ_q, $q=1,\ldots,n$, and we wish to solve for $|\psi_1\rangle$. According to the usual degenerate perturbation theory, V is diagonalized with respect to the ϕ_q to give the correct zero-order eigenfunctions $\psi_q^{(0)}$, $q=1,\ldots,n$, such that

$$\langle\psi_q^{(0)}\,|\,V\,|\,\psi_{q'}^{(0)}\rangle=E_q^{(1)}\delta_{qq'},\quad q,q'=1,\ldots,n \tag{15}$$

where $E_q^{(1)}$ is the first-order energy for the state $|\psi_q\rangle$. Unlike the nondegenerate case, Eq. (11) no longer completely defines $|\psi_1^{(s)}\rangle$, to which may be added arbitrary multiples of the degenerate states:

$$|\psi_1^{(s)}\rangle=|\chi_1^{(s)}\rangle+\sum_{q=1}^{n}b_{1q}^{(s)}\,|\psi_q^{(0)}\rangle\ , \tag{16}$$

where $|\chi_1^{(s)}\rangle$ is defined by Eq. (11) and $b_{1q}^{(s)}$ is the s-order mixing coefficient of $|\psi_1^{(s)}\rangle$ with the qth state. The s-order equation for the state $|\psi_1\rangle$ is

$$(H_0-E_1^{(0)})\,|\psi_1^{(s)}\rangle=-(V-E_1^{(1)})\,|\psi_1^{(s-1)}\rangle+\sum_{r=2}^{s}E_1^{(r)}\,|\psi_1^{(s-r)}\rangle\ . \tag{17}$$

In order that this equation be mathematically consistent its right-hand side must be orthogonal to each of the n eigenfunctions $\psi_q^{(0)}$. One of the conditions, that $\psi_1^{(0)}$ is orthogonal to the right-hand side, is used to determine the s-order energy $E_1^{(s)}$. Multiplying Eq. (17) by $\psi_1^{(0)*}$ and integrating gives

$$E_1^{(s)}=\langle\psi_1^{(0)}\,|\,V\,|\,\psi_1^{(s-1)}\rangle-\sum_{r=1}^{s-1}E_1^{(r)}\langle\psi_1^{(0)}\,|\,\psi_1^{(s-r)}\rangle\ , \tag{18}$$

which is identical in form to Eq. (12).

The other $n-1$ conditions are used to determine $\psi_1^{(s-1)}$, i.e., to determine the mixing coefficients $b_{1q}^{(s-1)}$, $q=2,\ldots,n$ ($b_{11}\equiv 0$ as will be shown below). Multiplying Eq. (17) by $\psi_q^{(0)*}$ and integrating we obtain

$$\langle\psi_q^{(0)}\,|\,V\,|\,\psi_1^{(s-1)}\rangle=\sum_{r=1}^{s}E_1^{(r)}\langle\psi_q^{(0)}\,|\,\psi_1^{(s-r)}\rangle,\quad s=2,\ldots,\infty$$

$$\left\langle\psi_q^{(0)}\middle|\,V\,\middle|\,\chi_1^{s-1}+\sum_{q'=1}^{n}b_{1q'}^{(s-1)}\psi_{q'}^{(0)}\right\rangle=\sum_{r=1}^{s}E_1^{(r)}\left\langle\psi_q^{(0)}\middle|\,\chi_1^{(s-r)}+\sum_{q'=1}^{n}b_{1q'}^{(s-r)}\psi_{q'}^{(0)}\right\rangle\ . \tag{19}$$

Using Eq. (15)

$$\langle\psi_q^{(0)}\,|\,V\,|\,\chi_1^{(s-1)}\rangle+b_{1q}^{(s-1)}E_q^{(1)}=\sum_{r=1}^{s}E_1^{(r)}b_{1q}^{(s-r)}\ , \tag{20}$$

so

$$b_{1q}^{(s-1)}=\frac{\langle\psi_q^{(0)}\,|\,V\,|\,\chi_1^{(s-1)}\rangle-\sum_{r=2}^{s-1}E_1^{(r)}b_{1q}^{(s-r)}}{E_1^{(1)}-E_q^{(1)}},\quad s=2,\ldots,\infty$$

$$b_{11}^{(s-1)}\equiv 0\ . \tag{21}$$

Having determined $\psi_1^{(s-1)}$ one can then solve for $E_1^{(s)}$ (or $E_1^{(2s-2)}$ and $E_1^{(2s-1)}$ using Wigner's rule) and continue iterating.

The oscillator strength for a dipole transition from ψ_n to $\psi_{n'}$ is given (in atomic units) in the length formulation by

$$f_l=\tfrac{2}{3}(E_{n'}-E_n)\left|\langle\psi_n\,|\sum_{i=1}^{4}\vec{r}_i\,|\,\psi_{n'}\rangle\right|^2\ , \tag{22}$$

and in the velocity formulation by

$$f_v=\tfrac{2}{3}(E_{n'}-E_n)^{-1}\left|\langle\psi_n\,|\sum_{i=1}^{4}\vec{\nabla}_i\,|\,\psi_{n'}\rangle\right|^2\ . \tag{23}$$

Using Eqs. (3) and (4) Z expansions of the oscillator strengths may be calculated:

$$f_l=\sum_{s=0}^{\infty}Z^{-s}f_l^{(s)}\ , \tag{24}$$

$$f_v=\sum_{s=0}^{\infty}Z^{-s}f_v^{(s)}\ . \tag{25}$$

If the eigenfunctions are exact, the coefficients of the length and velocity expansions are identical.

III. CALCULATIONS AND RESULTS

The diagonalization of H_0 to obtain the zero-order basis set ϕ_k and the calculation of the matrix elements $\langle \phi_{k'} | V | \phi_k \rangle$ were done by modifying a configuration-interaction program written by Schaefer.[5] This program uses L-S configurations of the form

$$\Phi = \sum_j b_j D_j \, ,$$

where b_j is a symmetry-adapted coefficient and D_j is a determinant of atomic orbitals. The atomic orbitals θ_i are of the general form

$$\theta_i = R_i Y_{l_i m_i}(\theta, \phi) \left\{ {\alpha \atop \beta} \right\} .$$

The radial function R_i is expanded as a sum of Slater-type orbitals,

$$R_i = \sum_k a_{ik} \chi_k \, , \quad \chi_k = \frac{(2\zeta)^{n+1/2}}{[(2n)!]^{1/2}} r^{n-1} e^{-\zeta r} ,$$

where ζ is the orbital exponent and n, l, m are the usual quantum numbers. These atomic orbitals are orthogonalized at the beginning of the program and remain fixed during the calculation. Hydrogenic orbitals are used for the $1s$, $2s$, and $2p$ orbitals instead of Hartree-Fock orbitals to ensure the correct values for the zeroth- and first-order coefficients in the Z expansion. This resulted in some loss of accuracy at low Z, but ensured that the series limit for high Z was correct. The remaining orbital exponents were guessed and no attempt was made to search for an optimum set. The final wave function for each state consists of 60 configurations.

The values for the orbital exponents and the configurations used for the ${}^1S$ and ${}^1P$ states are shown in Tables I and II. Using these basis sets the wave functions and energies for the $1s^22s^2\ {}^1S$, $1s^22p^2\ {}^1S$, and the $1s^22s2p\ {}^1P$ states of the entire beryllium isoelectronic sequence were obtained

TABLE I. Atomic orbitals and configurations of the $1s^22s^2$ and the $1s^22p^2\ {}^1S$ states.

Atomic orb.	Slater orb. n	 l	Scaled orb. exp.	Configurations	
$1s$	1	0	1.0000	$1s^22s^2$	$1s^22p3p$
$2s$	2	0	0.5000	$1s^22p^2$	$1s^23d^2$
	1	0	0.5000	$1s^22s1s'$	$1s^23d'^2$
$1s'$	1	0	0.3675	$1s^22s1s''$	$1s^23d3d'$
$1s''$	1	0	1.5874	$1s^22s2s'$	$2s^21s'^2$
$2s'$	2	0	0.9250	$1s^22s2s''$	$2s^21s''^2$
$2s''$	2	0	0.3675	$1s2s^21s'$	$2s^21s'1s''$
$3s$	3	0	0.4500	$1s2s^21s''$	$2s^21s'2s'$
				$1s2s^22s'$	$2s^22p^2$
$2p$	2	1	0.5000	$1s^21s'^2$	$2s^22p'^2$
$2p'$	2	1	0.6875	$1s^22s'^2$	$2s^22p''^2$
$2p''$	2	1	1.2125	$1s^21s'1s''$	$2s^22p2p'$
$2p'''$	2	1	0.2840	$1s^21s'3s$	$2s^22p2p''$
$3p$	3	1	1.2125	$1s^21s'2s''$	$2s^22p'2p''$
$3p'$	3	1	0.4875	$1s^21s''2s'$	$2s^23d^2$
$3d$	3	2	1.1125	$1s^22s'2s''$	$2s^23d3d'$
$3d'$	3	2	0.4625	$1s^21s''^2$	$1s2s1s'^2$
				$1s^22s''^2$	$1s2s2s'^2$
				$1s2s^22s''$	$1s2s1s'2s'$ (2)
				$1s^21s''2s''$	$1s2s1s'1s''$ (2)
				$1s^22p'^2$	$1s2s2p^2$
				$1s^22p''^2$	$1s2s2p'^2$
				$1s^22p'''^2$	$1s2s2p''^2$
				$1s^22p2p'$	
				$1s^22p2p''$	$1s2s2p2p'$ (2)
				$1s^22p2p'''$	
				$1s^22p'2p''$	$1s2s2p2p''$ (2)
				$1s^22p'2p'''$	$1s2s3d^2$
				$1s^22p''2p'''$	
				$1s^22p3p$	

TABLE II. Atomic orbitals and configurations of the $1s^22s2p\ ^1P$ state.

	Slater orb.				
Atomic orb.	n	l	Scaled orb. exp.	Configurations	
				$1s^22s2p$	$1s^23p3d$
$1s$	1	0	1.0000	$1s^22s2p'$	$1s^23p3d'$
$2s$	2	0	0.5000	$1s^22s2p''$	$2s2p1s'^2$
	1	0	0.5000	$1s^22s3p$	$2s2p2p'^2$ (2)
$1s'$	1	0	1.4772	$1s^22p1s'$	$2s2p^22p'$ (3)
$2s'$	2	0	0.7498	$1s^22p1s''$	$1s2p2p'^2$
$3s$	3	0	0.4125	$1s^22p2s'$	$1s2s^22p$
$1s''$	1	0	0.8700	$1s^22p2s''$	$1s2s^22p''$
$2s''$	2	0	0.3682	$1s^22p3s$	$1s2s^23p$
$3s'$	3	0	0.3500	$1s^22p3d$	$1s2p^22p'$ (3)
$2p$	2	1	0.5000	$1s^22p3d'$	$1s2p^23p$ (3)
$2p'$	2	1	1.5268	$1s2s2p1s'$	$1s2p1s'2s'$
$3p$	3	1	0.3525	$1s2s2p1s''$	$1s2p1s'3s$
$2p''$	2	1	0.3591	$1s2s2p2s'$	$1s2p2s'3s$
$3p'$	3	1	0.9800	$1s2s2p3s$	$1s2s1s'2p'$ (2)
$2p'''$	2	1	0.6500	$1s2s2p3d$ (2)	$1s2s1s'3p$ (2)
$3d$	3	2	0.4025	$1s2s2p3d'$ (2)	$1s2s2s'3p$ (2)
$3d'$	3	2	1.1000	$1s^21s'2p'$	$1s2p1s'3d$
				$1s^21s'2p''$	$1s2s2p'3d$
				$1s^21s'3p$	$1s2s3p3d$
				$1s^22s'2p'$	
				$1s^22s'2p''$	
				$1s^22s'3p$	
				$1s^23s2p'$	
				$1s^23s2p''$	
				$1s^23s3p$	
				$1s^22p'3d$	
				$1s^22p''3d$	

using Eqs. (13), (14), and (16). Table III shows a comparison of the eigenvalues obtained for the series with some variational calculations of Weiss[6] and Hibbert.[7] The eigenvalues obtained are understandably unable to compete in accuracy with those more refined calculations for which orbital exponents were optimized at each Z value; our accuracy at each Z value could be considerably

TABLE III. Eigenvalues (a.u.) for the beryllium isoelectronic sequence.

	$1s^22s^2\ ^1S$		$1s^22s2p\ ^1P$		$1s^22p^2\ ^1S$	
Z	Z expansion	Weiss (Ref. 6)	Z expansion	Hibbert (Ref. 7)	Z expansion	Hibbert (Ref. 7)
5	−24.3099	−24.3413	−23.9324	−23.9571	...	
6	−36.5036	−36.5262	−35.9998	−36.0054	−35.5692	−35.6417
7	−51.1951	−51.2128	−50.5648	−50.5647	−50.0218	−50.0871
8	−68.3858	−68.4001	−67.6295	−67.6215	−66.9735	−67.0366
9	−88.0761		−87.1946		−86.4257	−86.4873
10	−110.2664		−109.2599		−108.3787	
11	−134.9567		−133.8255		−132.8326	
12	−162.1470		−160.8913		−159.7872	
13	−191.8374		−190.4573		−189.2424	
14	−224.0278		−222.5235		−221.1981	

TABLE IV. Energy-expansion coefficients $E_n^{(s)}$ (Z^2 a.u.).

Order	$1s^22s^2\ {}^1S$	$1s^22s2p\ {}^1P$	$1s^22p^2\ {}^1S$
0	−1.250 000 00(0)	−1.250 000 00(0)	−1.250 000 00(0)
1	1.559 274 21(0)	1.682 737 60(0)	1.790 576 00(0)
2	−8.523 933 49(−1)	−1.062 740 15(0)	−1.216 212 22(0)
3	−7.906 534 38(−2)	−3.347 332 77(−1)	−6.957 087 26(−1)
4	4.266 424 46(−2)	1.053 643 59(0)	−4.064 794 68(−1)
5	1.909 615 45(−1)	−4.805 613 86(−1)	3.308 446 02(0)
6	3.852 019 09(0)	−1.344 859 10(1)	2.253 794 97(1)
7	1.289 291 95(1)	−6.042 041 91(0)	8.028 664 24(0)
8	3.830 020 30(0)	1.995 529 51(2)	−3.102 491 07(2)
9	−8.442 240 86(1)	7.194 578 01(2)	−4.974 855 44(2)
10	−3.348 991 36(2)	4.994 929 90(2)	6.675 719 93(3)

improved with a single optimization of the scaled exponents used for the entire series. It should be emphasized also that within the same basis set, the Z-expansion results are identical to the results obtained by diagonalizing the full Hamiltonian for each value of Z. Note that the series does not converge below $Z=5$. The agreement with the variational calculations of Weiss and Hibbert increases as Z increases. Results are given through $Z=14$, Si XI, beyond which relativistic effects become important. Table IV shows the energy-expansion coefficients for the three states.

The energy for the lowest ${}^1S$ state is given to second order by $E=-1.25Z^2+1.559\,274Z-0.852\,393$. The Z expansion of the Hartree-Fock energy to second order is[8] $E^{\text{HF}}=-1.25Z^2+1.571\,001Z-0.805\,468$, giving $E^{\text{corr}}=-0.0117\,27Z-0.046\,925$ for the correlation energy. The semiempirical values for $E^{(2)}$ of −0.880 (Ref. 9) and −0.875 (Ref. 10) suggest that our value of $E^{(2)}$ has not converged. A larger calculation using 150 configurations resulted in a value for $E^{(2)}$ of −0.861 33.

The dipole length and velocity values for the $2s^2\ {}^1S$-$2s2p\ {}^1P$ and the $2s2p\ {}^1P$-$2p^2\ {}^1S$ transitions

TABLE V. Comparison of oscillator strengths calculated by the Z-expansion method with other works for the $1s^22s^2\ {}^1S$-$1s^22s2p\ {}^1P$ transition.

		Z expansion	Ref. 7	Ref. 13	Ref. 14	Ref. 15	Ref. 16	Ref. 17	Ref. 18
C III	f_l	0.777	0.788	0.760	0.787	0.770	0.840	0.765	0.764
	f_v	0.803	0.756	0.780		0.843			
N IV	f_l	0.634	0.625	0.605	0.644		0.679		0.614
	f_v	0.651	0.580	0.631					
O V	f_l	0.530	0.524	0.513	0.543	0.517	0.569	0.515	0.513
	f_v	0.548	0.498	0.525		0.570			
F VI	f_l	0.456		0.435					
	f_v	0.473		0.464					
Ne VII	f_l	0.399		0.384	0.416		0.432		
	f_v	0.417		0.408					
Na VIII	f_l	0.356			0.373				
	f_v	0.372							
Mg IX	f_l	0.321			0.339				
	f_v	0.336							
Al X	f_l	0.293							
	f_v	0.306							
Si XI	f_l	0.269		0.261	0.287				
	f_v	0.281		0.265					

TABLE VI. Comparison of oscillator strengths calculated by the Z-expansion method with other works for the $1s^22s2p\ {}^1P$-$1s^22p^2\ {}^1S$ transition.

		Z expansion	Ref. 7	Ref. 13	Ref. 14	Ref. 15	Ref. 16
C III	f_l	0.142	0.166	0.173	0.207	0.17	0.158
	f_v	0.159	0.168	0.163			
N IV	f_l	0.122	0.136	0.135	0.158		0.128
	f_v	0.140	0.138	0.144			
O V	f_l	0.107	0.116	0.112	0.130	0.11	0.108
	f_v	0.121	0.118	0.129			
F VI	f_l	0.094	0.101	0.101			
	f_v	0.106	0.104	0.111			
Ne VII	f_l	0.084	0.090	0.092	0.116		0.083
	f_v	0.095	0.091	0.096			
Na VIII	f_l	0.077			0.085		
	f_v	0.083					
Mg IX	f_l	0.071			0.077		
	f_v	0.075					
Al X	f_l	0.065					
	f_v	0.068					
Si XI	f_l	0.061		0.062	0.064		
	f_v	0.062		0.064			

are listed in Tables V and VI and compared with various other calculations. Experimental energy differences are used so that the inaccuracies in the calculation are due to the transition integral alone. The energy differences used were obtained from Moore[11] for $Z = 6-8$ and from Wiese *et al.*[12] for $Z = 9-14$. For the $2s^2$-$2s2p$ transition the length values seem to be in better agreement with other calculations although the length and velocity results agree to within 5%. The length and velocity results for the $2s2p$-$2p^2$ transition disagree by as much as 15% for low-Z values, the disagreement reducing to 5% for $Z \geq 12$. This is due in large part to the eigenfunction of the $1s^22p^2\ {}^1S$ state, which is not as accurate as the eigenfunctions of the other two states which are the lowest states of their respective symmetries. The agreement with experiment is good for both transitions as noted by Nicolaides *et al.*[13] The expansion coefficients for the square of the transition integral and for the oscillator strength with calculated energy differences are given in Tables VII–X.

TABLE VII. Z-expansion coefficients for the $2s^2\ {}^1S$-$2s2p\ {}^1P$ transition in the length formulation .

Order	$T_l = \frac{1}{Z^2}\sum_{s=0}^{\infty} Z^{-s} T_l^{(s)}$ Transition element squared	$f_l = \sum_{s=0}^{\infty} Z^{-s} f_l^{(s)}$ Oscillator strength (with calculated ΔE)
0	1.283 181 86(1)	0.00
1	4.977 757 96(1)	3.168 519 73(0)
2	1.831 721 91(2)	6.893 153 78(0)
3	5.387 997 66(2)	1.772 764 22(1)
4	1.885 924 00(3)	5.647 707 11(1)
5	5.766 588 54(3)	2.287 675 15(2)
6	−2.531 994 48(3)	2.145 378 24(2)
7	−1.229 713 05(5)	−5.380 407 52(3)
8	−6.011 624 16(5)	−3.235 884 34(4)
9	−1.532 811 57(6)	−7.175 236 99(4)
10	−1.955 722 12(6)	1.191 458 26(4)

TABLE VIII. Z-expansion coefficients for the $2s^2\ {}^1S$-$2s2p\ {}^1P$ transition in the velocity formulation .

Order	$T_v = Z^2\sum_{s=0}^{\infty} Z^{-s} T_v^{(s)}$ Transition element squared	$f_v = \sum_{s=0}^{\infty} Z^{-s} f_v^{(s)}$ Oscillator strength (with calculated ΔE)
0	0.0	0.0
1	0.0	3.661 668 16(0)
2	2.260 409 89(−1)	3.861 906 94(0)
3	−1.467 080 27(−1)	−5.677 136 57(0)
4	−1.224 714 73(0)	1.400 222 69(1)
5	2.818 717 55(0)	4.536 826 44(2)
6	2.798 237 55(1)	1.182 516 72(3)
7	−1.234 750 35(1)	−5.170 712 15(3)
8	−5.606 514 93(2)	−3.675 260 58(4)
9	−1.280 632 01(3)	−5.830 878 14(4)
10	3.154 637 83(3)	9.109 001 62(4)

TABLE IX. Z-expansion coefficients for the $2s2p\ {}^1P$-$2p^2\ {}^1S$ transition in the length formulation .

Order	$T_l = \frac{1}{Z^2}\sum_{s=0}^{\infty} Z^{-s} T_l^{(s)}$ Transition element squared	$f_l = \sum_{s=0}^{\infty} Z^{-s} f_l^{(s)}$ Oscillator strength (with calculated ΔE)
0	1.116 818 14(1)	0.0
1	3.523 053 58(1)	8.029 058 30(−1)
2	6.343 386 51(1)	1.390 133 67(0)
3	1.254 523 54(2)	−1.731 824 21(0)
4	1.118 646 03(3)	−1.682 068 25(1)
5	8.097 762 95(3)	4.623 793 04(1)
6	3.144 352 30(4)	7.327 035 58(2)
7	8.921 579 62(3)	2.150 919 77(3)
8	−7.650 933 58(5)	−7.239 870 80(3)
9	−5.595 444 53(6)	−8.597 043 48(4)
10	−2.007 113 09(7)	−3.124 308 97(5)

TABLE X. Z-expansion coefficients for the $2s2p\ {}^1P$-$2p^2\ {}^1S$ transition in the velocity formulation.

Order	$T_v = Z^2\sum_{s=0}^{\infty} Z^{-s} T_v^{(s)}$ Transition element squared	$f_v = \sum_{s=0}^{\infty} Z^{-s} f_v^{(s)}$ Oscillator strength (with calculated ΔE)
0	0.0	0.0
1	0.0	7.030 068 59(−1)
2	1.137 166 95(−1)	1.479 255 82(0)
3	7.744 298 40(−2)	5.809 819 64(0)
4	2.185 934 30(−1)	−1.726 269 68(1)
5	−6.470 517 12(0)	−2.465 490 17(2)
6	−3.829 726 16(1)	−6.726 129 31(2)
7	−9.064 585 12(0)	7.824 359 90(2)
8	5.804 194 39(2)	9.119 275 34(3)
9	1.908 301 87(3)	1.102 173 80(4)
10	−3.891 944 61(3)	−1.245 205 00(5)

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