

## ACCURATE WAVEFUNCTION FOR ATOMIC BERYLLIUM

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We describe the most accurate to date configuration-interaction wavefunction for Be ground state  $\Psi = \sum \Phi_K^{(p)} a_{Kp}$  where  $\Phi_K^{(p)}$  is a  $LS$  eigenfunction for configuration  $K$  and electron coupling  $p$ . We present tables for the coefficients  $a_{Kp}$  associated with the invariant portions of the wavefunction. We also specify the electron couplings and phase factors of the  $\Phi_K^{(p)}$ 's and the orbital basis  $\psi_{ilm} = R_{il}(r) Y_{lm}(\theta, \phi)$  characterized by  $R_{il} = \sum S_{jl} a_{jli}$  and  $S_{jl} = N_{jl} r^{(n_j-1)} \exp(-Z_{jl}r)$ . Our wavefunction, after inclusion of approximate relativistic and radiative corrections, gives a total electronic energy for  ${}^9\text{Be}$  of  $-14.668\,451\,(28)$  a.u. in agreement with the latest experimental-theoretical value of  $-14.668\,452\,(2)$  a.u.

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## INTRODUCTION

*Preface*

Why another Be wavefunction when so many of them<sup>1</sup> are described in the literature? The answer is twofold: (i) The present wavefunction gives by far the lowest upper bound to the nonrelativistic energy<sup>2,3</sup> and permits estimation of a total electronic energy  $E = -14.668\,451\,(28)$  a.u. for  $\text{Be}^{2,3}$ , that is, with an uncertainty of 2 ppm, in remarkably good agreement with the latest experimental-theoretical value  $E = -14.668\,452\,(2)$  a.u.<sup>2</sup> and (ii) All energy and wavefunction truncation errors are known with a good amount of detail,<sup>3</sup> orders of magnitude better than in any other previous work.

The nonrelativistic wavefunction tabulated here has been determined by the standard configuration-interaction (CI) method<sup>4</sup> in an attempt to make an accurate numerical test<sup>2</sup> of atomic-structure theory for a small many-electron system. It can be used in at least three ways:

(i) To set up well-defined sequences of truncated wavefunctions. These may be used to find corresponding sequences of expectation values, presumably converging towards their exact values, except for a small margin of error due to the finite size of the Slater-type orbital basis. These sequences can also be used in stability studies of

mathematical details of the wavefunction, such as the behavior of the  $p^{\text{th}}$ -order reduced-density matrices for particularly interesting values of the electronic coordinates, or for testing more subtle aspects of the theory of partial differential equations.

(ii) To permit an appreciation of what an accurate atomic wavefunction looks like when expressed in an orthogonal basis (in an orthogonal basis only approximate localization can be achieved; even when localized orbitals are used, it is found<sup>3</sup> that the  $K$ ,  $L$ , and intershell ( $I$ ) portions of the wavefunction extend over regions of space well beyond any intuitively reasonable limits when microhartree order of accuracy is involved).

(iii) As a benchmark either to facilitate improved calculations or to interpret the deficiencies of less accurate wavefunctions.

*The Standard Atomic CI Method*

In the standard CI method,<sup>4</sup> the solution to the nonrelativistic Schrödinger equation with Hamiltonian

$$H = \sum_{i=1}^N \{ -(1/2)\nabla_i^2 - Z/r_i \} + \sum_{i<j} 1/r_{ij} \quad (1)$$

is approximated by a finite expansion

$$\Psi = \sum \Phi_K^{(p)} a_{Kp} \quad (2)$$

based on (i)  $LS$  eigenfunctions  $\Phi_K^{(p)}$ , (ii) orthogonal one-electron symmetry-adapted spin-orbitals with equivalence of partner orbitals in degenerate representations, and (iii) Slater-type orbital (STO) basis.

The  $LS$  eigenfunctions (or configuration state functions, or terms) are obtained as successively orthogonalized symmetric projections<sup>5</sup> of Slater determinants. They may be expressed as linear combinations of Slater determinants

$$\Phi_K^{(p)} = \sum_{\alpha=p}^{n_K} D_{K\alpha} c_{K\alpha}^{(p)}, \quad (3)$$

or, in projected form:

$$\Phi_K^{(p)} = O(L^2, S^2) \sum_{\alpha=1}^p D_{K\alpha} b_{K\alpha}^{(p)}, \quad (4)$$

where  $O(L^2, S^2)$  is an idempotent projection operator for  $L^2$  and  $S^2$  and the superscript  $p$  is used to distinguish the elements of a possibly degenerate configuration  $K$ . It has been demonstrated<sup>6,7</sup> that when degeneracies exist, the different  $LS$  eigenfunctions of configuration  $K$  given by Eq. (4) may be chosen so that they are characterized by internal couplings of electron groups and an arbitrary phase factor. An extensive theoretical discussion<sup>7</sup> and computational details<sup>8</sup> are given in the literature.

The spin-orbitals  $\psi_{ilms}$  are expressed as linear combinations of normalized STO's  $S_{jl}$ , times a normalized spherical harmonic in Dirac's phase convention,<sup>9</sup> times a usual spin function:

$$\psi_{ilms} = R_{il}(r) Y_{lm}(\theta, \phi)(\alpha \text{ or } \beta) \quad (5)$$

$$R_{il} = \sum S_{jl} a_{jli} \quad (6)$$

$$S_{jl} = N_{jl} r^{(n_j-1)} \exp(-Z_{jl}r). \quad (7)$$

We shall now explain how to find the parameters that determine the basis spin-orbitals and the linear coefficients  $a_{Kp}$  of Eq. (2).

### Current CI Techniques

The nonlinear parameters (orbital exponents)  $Z_{jl}$  of Eq. (7) are determined by sophisticated optimization techniques<sup>3</sup> which make use of preliminary studies of patterns of convergence for each harmonic in the  $K$ ,  $L$ , and  $I$  portions of the wavefunction.

The linear coefficients  $a_{jli}$  of Eq. (6) are determined by particular<sup>3</sup> natural orbital<sup>10</sup> (NO) transformations. The NO's are eigenfunctions of the reduced first-order density matrix; the corresponding eigenvalues are usually called occupation numbers. For  $^1S$  states these occupation numbers are independent of  $m$  and  $s$  and are usually denoted by  $n_{il}$ . It is customary to order the  $n_{il}$ 's in nonincreasing order, for each  $l$ , that is,  $n_{il} \geq n_{i+1,l}$ .

Here the subscript  $i$  is to be identified with the same subscript in Eqs. (5) and (6). For a given STO basis the  $a_{jli}$ 's largely determine the convergence of the truncated CI series towards the full CI expansion.

The matrix elements of the Hamiltonian are computed by means of well-established formulas.<sup>5,9</sup>

The eigenvector components or CI coefficients  $a_{Kp}$  of Eq. (2) are obtained by the method of optimal relaxation of Shavitt and coworkers.<sup>11</sup> The iterations are stopped when

$$|a_{Kp}^{(i+1)} - a_{Kp}^{(i)}| \leq 10^{-5} \quad (8)$$

for all  $a_{Kp}$ 's. Among all possible  $\Phi_K^{(p)}$ 's with given  $10s9p8d7f5g3h1i$  orbital basis, those with  $a_{Kp}$  absolute values larger than 0.0003 are believed to be included without exception. (This corresponds to the leading 253 coefficients of our 650-term CI expansion.)

It is possible to compute estimates  $\Delta E_m$  of energy contributions,<sup>12</sup> for  $\Phi_m \equiv \Phi_K^{(p)}$ :

$$\Delta E_m = a_m^2 (E - H_{mm}) / (1 - a_m^2). \quad (9)$$

These are useful in many ways.<sup>3</sup>

Beyond the 650 terms reported here the energy convergence towards the full CI in the given orbital basis is very slow; the estimate of the full CI energy is only  $-0.000\ 019\ (2)$  a.u. below the 650-term upper bound.<sup>3</sup>

The energy error due to the finite size of our orbital basis is estimated<sup>3</sup> as  $-0.000\ 407\ (23)$  a.u. This number is obtained as the sum of twenty smaller quantities associated with different invariant portions of the wavefunction.

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## EXPLANATION OF TABLES

$a_{j0i}, a_{j1i}$ , etc.	Linear coefficients of Eq. (6)
STO	Slater-type orbital
$s_3, p_1$ , etc.	Third $s$ -orbital, first $p$ -orbital, etc.
$l_a$	Orbital with azimuthal quantum number $l$ and ordering number $a$
${}^3S(1s2s) \rightarrow {}^3S(l_a l_b)$ $+ ns\alpha d^2\alpha p_a^1\beta p_b^1\beta$	Means ${}^1S[{}^3S(1s2s){}^3S(l_a l_b)]$ Ordered spin-orbital product corresponding to the main diagonal of a Slater determinant. It occurs with + sign thus specifying the phase of the corresponding configuration state function given by Eqs. (3) and (4)
$p_a^{\bar{1}}\alpha$	Spin-orbital with $i = a, l = 1, m = -1, s = +1/2$
${}^1S(l_a l_b)$	Orbitals $l_a$ and $l_b$ coupled into a ${}^1S$ state
EIGENVEC	Configuration-interaction (CI) coefficient $a_m = a_{Kp}$ , Eq. (2)
ENERGY	Energy contribution $-\Delta E_m$ , Eq. (9), in $10^{-6}$ a.u. = $0.219 \text{ cm}^{-1}$ . The results were originally obtained in a.u. (Be) and then converted into a.u. based on Ref. 13: $R_\infty = 109\,737.3177 (83) \text{ cm}^{-1}$ $R({}^9\text{Be}) = 109\,730.6377 (83) \text{ cm}^{-1}$

## Notes for Tables 2-11

In Table 2 the subscripts satisfy  $a \leq b$   
 In Table 3 the subscripts satisfy  $a \leq b \leq c \leq d$  whenever they are related.  
 Also,  $l \leq l'$ ; the primes have been deleted in the second column;  $n = 1$  or 2

EXPLANATION OF TABLES, continued

		Example		
		Orbital Coefficients $a_{j5i}$ , Eq. (6)		
	h	$h_1$	$h_2$	$h_3$
	Slater-type orbital set			
6h	2.400	1.0000259	-0.0076335873	0.0081948631
6h	15.500	-0.0054219565	1.5837405	-2.1515391
7h	22.000	0.0042547375	-0.66322899	2.5878929
$n_j, l$	Orbital exponents	$R_{i1} = R_{15}$	$R_{25}$	$R_{35}$
	$Z_{j1} = Z_{j5}$	Expansion coefficients	Expansion coefficients	Expansion coefficients

Description of orbitals of  $h$ -symmetry

Therefore,

$$R_{15} = N_{15}[r^{6-1} \exp(-2.400r)] 1.0000259 + N_{25}[r^{6-1} \exp(-15.500r)] (-0.0054219565) + N_{35}[r^{7-1} \exp(-22.000r)] 0.0042547375$$

where

$$N_{j1} = (2Z_{j1})^{(n_j+1/2)} / [(2n_j)!]^{1/2}$$

TABLE 1 (1). ORBITAL BASIS

s		Orbital Coefficients $a_{j0i}$				
STO Set	$1s$	$2s$	$3s$	$4s$	$5s$	
1s 6.225	0.097245498	-0.0063789596	0.40481639	1.7134019		
1s 3.437	0.91682650	-0.18627325	-0.34914771	-2.4630394		
3s 1.776	-0.021424131	0.73889522	-2.5307959	0.66681511		
2s 0.869	-0.0099914201	0.30051883	1.4982775	-1.1797614		
3s 1.080	0.0017458338	0.33063615	0.24400016	0.10943926		
4s 2.700	0.012760238	-0.16614308	0.28706684	0.47945211		
5s 2.200	0.0062535551	-0.15577729	0.48474186	0.34930920		
2s 7.450	0.0005805742	0.0034566694	0.17223739	0.82821611		
3s 8.800	-0.0008773940	0.0048859999	0.020650625	-0.029129174		
4s 16.000	-0.0004181908	-0.0009044007	0.0028055538	0.035567455		
	$s_5$	$s_6$	$s_7$	$s_8$		
	-0.97852527	0.88037959	4.3948621	8.9339738		
	0.74745545	-4.3216603	-13.543984	-18.160660		
	-3.8355048	-8.8054206	87.961668	89.478313		
	-3.0726619	2.9526406	-3.2687597	-30.053663		
	0.93670440	-0.60923782	-0.52381825	23.287274		
	1.4739106	6.8799815	-49.866476	-43.040204		
	4.5010038	0.57511383	-36.478405	-39.799130		
	-0.74038433	-0.21994932	1.9070289	2.3232270		
	1.6403279	3.8051268	2.7334033	8.9812850		
	-0.15950549	-0.14305796	1.5816663	-4.3815482		
	$s_9$	$s_{10}$				
	-16.061055	1.8287121				
	35.616097	20.165117				
	-121.50693	-66.463230				
	-71.407500	-14.438074				
	65.211132	14.251287				
	82.960819	39.468552				
	50.190299	28.741252				
	-3.5343442	-38.872456				
	-12.406198	11.517032				
	3.6788749	10.124911				
p		Orbital Coefficients $a_{j1i}$				
STO Set	$p_1$	$p_2$	$p_3$	$p_4$		
2p 1.036	1.0196298	-0.23492489	-1.4828457	1.9643744		
4p 5.000	-0.0041778551	-1.1994430	1.2880545	2.0462113		
3p 2.100	-0.093292910	-1.0974206	2.2600296	-1.7772088		
6p 2.800	0.067114425	0.44877460	-0.36542216	-0.68542390		
2p 2.900	0.0036990286	2.6520204	-1.5018638	-1.3507632		
3p 14.900	0.0012827277	0.013340864	-0.10487941	-0.42337093		
4p 14.000	-0.0017302782	0.0084395548	0.11396052	0.56162624		
5p 14.000	0.0031224121	0.050506102	-0.28947509	-1.1732073		
6p 14.000	-0.0008967434	-0.023391713	0.16197063	0.72496892		
	$p_5$	$p_6$	$p_7$	$p_8$		
	-2.3744815	-2.1194232	-1.2727858	-0.87883943		
	-0.94973019	3.3268596	16.086988	28.063550		
	-2.1172915	-4.4651407	2.8299517	10.810786		
	3.6298097	4.8735947	0.95212020	-2.8244945		
	2.4316133	0.20575324	-19.751025	-39.961294		
	-1.1630977	1.3673217	-0.24529108	10.600088		
	1.5377115	-1.7673707	0.44904368	-22.795640		
	-2.8393932	1.9021464	6.8564483	26.832198		
	1.8711626	-2.2479936	-2.7356824	-3.2096850		
	$p_9$					
	-0.96838532					
	73.328693					
	36.981172					
	-13.194229					
	-113.56638					
	0.79180953					
	40.133296					
	-55.401277					
	48.884758					

See pages 296-297 for Explanation of Tables

TABLE 1 (2). ORBITAL BASIS

d		Orbital Coefficients $a_{j2i}$			
STO Set	$d_1$	$d_2$	$d_3$	$d_4$	
3d 1.600	-0.44111041	-1.1011134	-1.6926754	-5.4151352	
4d 1.740	1.4008848	0.89275137	3.5564940	0.60373476	
5d 2.550	0.020482872	0.20570687	-2.1115601	4.8405499	
3d 7.100	0.035875876	-0.93153776	0.27193337	-0.46361019	
4d 16.000	-0.018445891	0.086472401	0.083364570	0.61655464	
5d 16.000	0.025138068	-0.092568507	-0.092121444	-0.44331818	
6d 16.000	-0.029822955	0.064972047	0.16930071	0.97705774	
3d 16.000	0.0009644042	0.020846694	-0.013783315	0.0002154239	
f		Orbital Coefficients $a_{j3i}$			
STO Set	$f_1$	$f_2$	$f_3$	$f_4$	
4f 1.560	0.52533917	-0.94499552	-2.6404912	-0.49175132	
5f 2.400	0.59154953	0.92532722	2.7773430	0.69840886	
4f 10.000	0.13511213	1.3150270	-0.50203573	-2.1302629	
5f 17.000	-0.12393373	-0.71958599	0.26430343	2.2396358	
6f 18.000	0.18415036	0.83887466	-0.32653794	-1.7634051	
7f 18.500	-0.17058682	-0.61338569	0.21451639	2.1954102	
4f 3.600	-0.20004677	0.072889948	-0.12052484	-0.38694807	
g		Orbital Coefficients $a_{j4i}$			
STO Set	$g_1$	$g_2$	$g_3$	$g_4$	
5g 1.900	0.87407278	-2.5491589	0.17502411	-0.067984745	
6g 2.800	0.13440512	2.6905018	-0.19880130	0.089144648	
5g 13.000	-0.022995359	0.069056218	1.5974151	-2.7854313	
6g 20.000	-0.0005230418	-0.029330875	-0.45128877	1.2492094	
7g 20.000	0.021024821	0.0041593934	-0.22834818	1.9572917	
h		Orbital Coefficients $a_{j5i}$			
STO Set	$h_1$	$h_2$	$h_3$		
6h 2.400	1.0000259	-0.0076335873	0.0081948631		
6h 15.500	-0.0054219565	1.5837405	-2.1515391		
7h 22.000	0.0042547375	-0.66322899	2.5878929		
i		Orbital Coefficients $a_{j6i}$			
STO Set	$i_1$				
7i 18.000	1.0000000				

See pages 296-297 for Explanation of Tables

TABLE 2. CHARACTERIZATION OF REFERENCE CONFIGURATION, SINGLE AND DOUBLE EXCITATIONS

Configuration	Phase Characterization of Determinants
$(1s)^2(2s)^2$	+ 1s $\alpha$ 2s $\alpha$ 1s $\beta$ 2s $\beta$
$2s \rightarrow s_a$	+ 1s $\alpha$ 2s $\alpha$ 1s $\beta$ s $_a\beta$
$(2s)^2 \rightarrow l_a l_b$	+ 1s $\alpha$ l $_a^0\alpha$ 1s $\beta$ l $_b^0\beta$
$^1S(1s2s) \rightarrow ^1S(l_a l_b)$	+ 1s $\alpha$ l $_a^0\alpha$ 2s $\beta$ l $_b^0\beta$
$^3S(1s2s) \rightarrow ^3S(l_a l_b)$	+ 1s $\alpha$ l $_a^0\alpha$ 2s $\beta$ l $_b^0\beta$
$(1s)^2 \rightarrow l_a l_b$	+ 2s $\alpha$ l $_a^0\alpha$ 2s $\beta$ l $_b^0\beta$

TABLE 3. CHARACTERIZATION OF TRIPLE AND QUADRUPLE EXCITATIONS

Configuration	Phase Characterization of Determinants
ns s $_a$ (s $_b$ ) <sup>2</sup>	+ ns $\alpha$ s $_b\alpha$ s $_a\beta$ s $_b\beta$
ns s $_b$ (s $_a$ ) <sup>2</sup>	+ ns $\alpha$ s $_a\alpha$ s $_a\beta$ s $_b\beta$
$^1S(ns s) ^1S(p_a p_b)$	+ ns $\alpha$ p $_a^0\alpha$ s $\beta$ p $_b^0\beta$
$^3S(ns s) ^3S(p_a p_b)$	+ ns $\alpha$ s $\alpha$ p $_a^0\beta$ p $_b^0\beta$
$^1D(ns d) ^1D(p_a p_b)$	+ ns $\alpha$ p $_a^1\alpha$ p $_b^1\beta$ d $^2\beta$
$^3D(ns d) ^3D(p_a p_b)$	+ ns $\alpha$ d $^2\alpha$ p $_a^1\beta$ p $_b^1\beta$
$^1P(ns p) ^1P(d f)$	+ ns $\alpha$ d $^0\alpha$ p $^0\beta$ f $^0\beta$
$^3P(ns p) ^3P(d f)$	+ ns $\alpha$ p $^0\alpha$ d $^0\beta$ f $^0\beta$
$^1P(ns p) ^1P(f g)$	+ ns $\alpha$ f $^0\alpha$ p $^0\beta$ g $^0\beta$
$^3P(ns p) ^3P(f g)$	+ ns $\alpha$ p $^0\alpha$ f $^0\beta$ g $^0\beta$
$^1S(l_a)^2 ^1S(l'_b)^2$	+ l $_a^0\alpha$ l $_b^0\alpha$ l $_a^0\beta$ l $_b^0\beta$
$^1S(l_a l_b) ^1S(l'_c)^2$	+ l $_a^0\alpha$ l $_c^0\alpha$ l $_b^0\beta$ l $_c^0\beta$
$^1S(l_a)^2 ^1S(l'_b l'_c)$	+ l $_a^0\alpha$ l $_b^0\alpha$ l $_a^0\beta$ l $_c^0\beta$
$^1S(l_a l_b) ^1S(l'_c l'_d)$	+ l $_a^0\alpha$ l $_c^0\alpha$ l $_b^0\beta$ l $_d^0\beta$
(p) <sup>4</sup> and (p $_a$ ) <sup>3</sup> p $_b$	+ p $_a^1\alpha$ p $_a^0\alpha$ p $_a^0\beta$ p $_b^1\beta$

TABLE 4. REFERENCE CONFIGURATION AND L SHELL SINGLE EXCITATIONS 2s  $\rightarrow$  s $_a$

a	EIGENVEC	ENERGY
3	-0.005 559	29
4	+0.002 380	45
5	+0.002 377	70
6	-0.001 592	64
8	+0.001 074	62
7	+0.951 (-3)	40
9	+0.814 (-3)	21
10	+0.26 (-4)	37 (-2)
$(1s)^2(2s)^2$	+0.9532844	1457 (+4)

See pages 296-297 for Explanation of Tables



TABLE 5. L SHELL DOUBLE EXCITATIONS  $(2s)^2 \rightarrow \ell_a \ell_b$

$\ell$	a b	EIGENVEC	ENERGY	$\ell$	a b	EIGENVEC	ENERGY	$\ell$	a b	EIGENVEC	ENERGY
0	3 3	-0.0393668	26(+2)	1	1 3	0.001 256	89(-1)	2	5 5	-0.222(-3)	48(-1)
0	3 4	0.009 565	84(+1)	1	5 5	-0.001 165	66	2	1 5	0.190(-3)	18(-1)
0	4 4	-0.003 477	20(+1)	1	2 2	0.930(-3)	13	2	4 6	0.163(-3)	32(-1)
0	5 5	-0.002 415	15(+1)	1	5 6	-0.795(-3)	41	2	5 6	-0.112(-3)	19(-1)
0	4 5	-0.002 362	12(+1)	1	1 6	0.580(-3)	14	2	2 2	0.64 (-4)	13(-2)
0	5 6	0.001 474	83	1	3 6	0.491(-3)	11	2	2 6	0.50 (-4)	29(-2)
0	6 6	-0.777(-3)	31	1	3 5	-0.456(-3)	62(-1)	2	2 5	0.43 (-4)	12(-2)
0	4 6	0.645(-3)	14	1	6 6	-0.427(-3)	15	2	4 7	0.42 (-4)	41(-2)
0	6 7	0.362(-3)	92(-1)	1	2 5	0.412(-3)	54(-1)	2	1 6	0.41 (-4)	17(-2)
0	3 5	-0.329(-3)	14(-1)	1	4 6	0.403(-3)	87(-1)	2	6 6	-0.41 (-4)	34(-2)
0	7 7	-0.267(-3)	63(-1)	1	2 6	0.342(-3)	56(-1)	2	5 7	-0.34 (-4)	30(-2)
0	3 6	0.255(-3)	17(-1)	1	3 7	-0.224(-3)	48(-1)				
0	4 7	0.236(-3)	29(-1)	1	5 7	-0.211(-3)	51(-1)	3	1 1	-0.006 110	97
0	7 8	-0.186(-3)	34(-1)	1	6 7	-0.181(-3)	43(-1)	3	3 3	-0.001 701	41
0	4 8	0.146(-3)	13(-1)	1	1 2	-0.169(-3)	20(-2)	3	2 3	-0.001 063	40
0	8 8	-0.146(-3)	23(-1)	1	1 7	0.114(-3)	12(-1)	3	2 2	-0.268(-3)	41(-1)
0	8 9	-0.103(-3)	91(-2)	1	2 7	0.73 (-4)	51(-2)	3	1 3	0.155(-3)	20(-2)
0	5 7	-0.97 (-4)	54(-2)	1	7 7	-0.56 (-4)	57(-2)	3	5 6	0.132(-3)	33(-1)
0	9 9	-0.96 (-4)	60(-2)	1	3 8	0.49 (-4)	43(-2)	3	5 5	-0.126(-3)	25(-1)
0	6 8	0.92 (-4)	67(-2)	1	6 8	-0.44 (-4)	42(-2)	3	1 2	0.97 (-4)	28(-2)
0	5 8	0.80 (-4)	42(-2)	1	5 8	-0.41 (-4)	34(-2)	3	2 4	-0.76 (-4)	57(-2)
0	6 9	-0.70 (-4)	28(-2)					3	6 6	-0.69 (-4)	11(-1)
0	5 9	0.59 (-4)	16(-2)	2	1 1	-0.0168637	40(+1)	3	4 6	0.62 (-4)	69(-2)
				2	3 3	-0.003 184	10(+1)	3	4 5	-0.59 (-4)	51(-2)
1	1 1	-0.2949222	44(+3)	2	3 4	0.001 366	51	3	5 7	0.23 (-4)	21(-2)
1	3 4	0.003 253	20(+1)	2	2 3	-0.928(-3)	18				
1	4 4	-0.002 568	18(+1)	2	4 4	-0.504(-3)	11	4	1 1	-0.002 861	31
1	3 3	-0.002 428	63	2	2 4	0.451(-3)	78(-1)	4	2 2	-0.001 178	78(-1)
1	1 4	-0.002 427	79	2	1 4	-0.425(-3)	41(-1)	4	2 3	0.90 (-4)	49(-2)
1	4 5	0.001 645	10(+1)	2	4 5	0.391(-3)	11	4	1 2	0.66 (-4)	20(-3)
1	2 3	0.001 568	31	2	1 2	-0.382(-3)	24(-1)				
1	1 5	0.001 500	55	2	3 5	-0.271(-3)	39(-1)	5	1 1	-0.001 554	14

TABLE 6. K SHELL DOUBLE EXCITATIONS  $(1s)^2 \rightarrow \ell_a \ell_b$

$\ell$	a b	EIGENVEC	ENERGY	$\ell$	a b	EIGENVEC	ENERGY	$\ell$	a b	EIGENVEC	ENERGY
0	4 4	-0.0152943	54(+2)	1	1 1	-0.993(-3)	10	2	7 7	-0.279(-3)	34
0	3 4	-0.0148730	37(+2)	1	5 6	0.976(-3)	69	2	2 5	-0.278(-3)	55(-1)
0	3 3	-0.008 120	73(+1)	1	6 6	-0.790(-3)	54	2	1 4	0.209(-3)	14(-1)
0	5 5	-0.001 957	13(+1)	1	1 4	-0.779(-3)	14	2	4 6	-0.172(-3)	38(-1)
0	5 6	-0.001 767	14(+1)	1	7 7	-0.526(-3)	51	2	3 5	-0.149(-3)	14(-1)
0	4 5	0.001 537	66	1	6 7	0.416(-3)	24	2	1 3	0.103(-3)	17(-2)
0	6 6	-0.001 172	79	1	2 5	-0.352(-3)	47(-1)	2	3 6	-0.93 (-4)	96(-2)
0	3 5	-0.763(-3)	13	1	1 5	-0.285(-3)	27(-1)	2	8 8	-0.82 (-4)	89(-1)
0	3 6	-0.722(-3)	18	1	4 6	0.274(-3)	46(-1)	2	6 7	0.62 (-4)	12(-1)
0	7 7	-0.511(-3)	25	1	8 8	-0.258(-3)	24	2	5 7	0.60 (-4)	98(-2)
0	6 7	-0.477(-3)	17	1	2 6	0.251(-3)	34(-1)	2	2 6	-0.31 (-4)	11(-2)
0	7 8	0.294(-3)	91(-1)	1	3 6	-0.217(-3)	25(-1)				
0	8 8	-0.232(-3)	62(-1)	1	4 7	0.212(-3)	49(-1)	3	2 2	-0.002 154	30(+1)
0	4 6	0.218(-3)	19(-1)	1	1 6	-0.126(-3)	77(-2)	3	2 3	0.001 140	57
0	4 7	-0.216(-3)	28(-1)	1	3 7	0.125(-3)	16(-1)	3	4 4	-0.001 001	14(+1)
0	8 9	0.212(-3)	42(-1)	1	9 9	-0.123(-3)	85(-1)	3	5 5	-0.430(-3)	30
0	9 9	-0.147(-3)	16(-1)	1	7 8	0.117(-3)	37(-1)	3	3 3	-0.341(-3)	28(-1)
0	3 7	0.146(-3)	11(-1)	1	2 7	0.82 (-4)	69(-2)	3	6 6	-0.274(-3)	17
0	5 8	-0.94 (-4)	65(-2)	1	6 8	0.78 (-4)	14(-1)	3	7 7	-0.171(-3)	18
0	10 10	-0.82 (-4)	71(-1)	1	3 8	0.45 (-4)	38(-2)	3	3 4	0.141(-3)	16(-1)
0	6 9	0.81 (-4)	43(-2)	1	4 8	0.41 (-4)	33(-2)	3	5 6	-0.116(-3)	26(-1)
0	5 7	0.66 (-4)	28(-2)	1	5 8	-0.40 (-4)	33(-2)	3	3 5	0.69 (-4)	45(-2)
0	4 9	0.50 (-4)	12(-2)	1	7 9	0.34 (-4)	43(-2)	3	4 5	0.68 (-4)	71(-2)
0	3 8	-0.46 (-4)	13(-2)	1	8 9	0.32 (-4)	46(-2)	3	1 2	-0.59 (-4)	13(-2)
								3	4 6	-0.36 (-4)	23(-2)
1	2 2	-0.0282939	17(+3)	2	2 2	-0.006 471	16(+2)	3	6 7	0.29 (-4)	35(-2)
1	1 2	-0.008 548	11(+2)	2	2 3	0.001 509	65	3	5 7	-0.24 (-4)	23(-2)
1	3 4	-0.003 296	29(+1)	2	4 4	-0.001 437	11(+1)				
1	3 3	-0.002 708	14(+1)	2	3 4	-0.001 039	38	4	3 3	-0.001 104	15(+1)
1	4 4	-0.002 511	22(+1)	2	4 5	-0.984(-3)	75	4	4 4	-0.492(-3)	63
1	2 3	0.001 964	77	2	5 5	-0.967(-3)	96	4	5 5	-0.215(-3)	25
1	4 5	-0.001 936	17(+1)	2	3 3	-0.582(-3)	66(-1)	4	2 3	-0.115(-3)	90(-2)
1	2 4	0.001 402	54	2	6 6	-0.569(-3)	66				
1	5 5	-0.001 352	10(+1)	2	1 2	0.559(-3)	76(-1)	5	2 2	-0.587(-3)	62
1	1 3	-0.001 136	19	2	2 4	0.504(-3)	11	5	3 3	-0.266(-3)	30
1	3 5	-0.001 110	46	2	5 6	0.296(-3)	14				
								6	1 1	-0.309(-3)	30

See pages 296-297 for Explanation of Tables

TABLE 7. INTERSHELL EXCITATIONS  $^1S(1s2s) \rightarrow ^1S(\ell_a \ell_b)$

$\ell$	a b	EIGENVEC	ENERGY	$\ell$	a b	EIGENVEC	ENERGY	$\ell$	a b	EIGENVEC	ENERGY
0	3 4	-0.005 454	36(+1)	1	6 7	0.128(-3)	22(-1)	3	2 5	-0.516(-3)	29
0	3 3	-0.004 972	14(+1)	1	6 6	-0.117(-3)	11(-1)	3	1 2	0.363(-3)	43(-1)
0	4 4	-0.004 744	43(+1)	1	7 7	-0.91(-4)	15(-1)	3	5 6	-0.355(-3)	24
0	3 5	-0.001 321	29	1	3 7	0.88(-4)	75(-2)	3	1 5	-0.340(-3)	96(-1)
0	5 5	-0.796(-3)	18	1	3 4	-0.66(-4)	96(-3)	3	5 5	0.340(-3)	18
0	5 6	-0.409(-3)	69(-1)	1	4 7	0.57(-4)	35(-2)	3	2 3	0.308(-3)	37(-1)
0	6 6	-0.273(-3)	40(-1)	1	3 6	0.56(-4)	15(-2)	3	1 3	0.295(-3)	11(-1)
0	4 5	-0.273(-3)	18(-1)	1	8 8	-0.54(-4)	10(-1)	3	1 4	-0.267(-3)	51(-1)
0	3 7	0.263(-3)	33(-1)	1	1 7	0.47(-4)	20(-2)	3	1 1	0.219(-3)	34(-2)
0	3 6	-0.217(-3)	14(-1)	1	2 7	0.44(-4)	19(-2)	3	3 5	-0.215(-3)	41(-1)
0	6 7	-0.121(-3)	11(-1)	1	7 8	0.42(-4)	48(-2)	3	2 6	0.213(-3)	64(-1)
0	4 7	0.114(-3)	72(-2)	1	5 7	-0.39(-4)	18(-2)	3	1 6	0.203(-3)	47(-1)
0	7 7	-0.97(-4)	86(-2)	1	9 9	-0.28(-4)	45(-2)	3	4 6	-0.201(-3)	73(-1)
0	7 8	0.94(-4)	90(-2)					3	2 2	0.198(-3)	24(-1)
0	3 9	-0.93(-4)	32(-2)	2	2 3	0.001 886	85	3	4 4	0.194(-3)	51(-1)
0	8 9	0.74(-4)	49(-2)	2	2 4	0.001 667	11(+1)	3	3 6	0.158(-3)	30(-1)
0	5 7	0.66(-4)	26(-2)	2	1 2	-0.001 441	40	3	6 6	0.103(-3)	24(-1)
0	4 8	0.58(-4)	22(-2)	2	1 3	-0.001 343	18	3	3 3	0.91(-4)	15(-2)
0	4 6	0.36(-4)	48(-3)	2	3 3	0.875(-3)	11	3	3 4	-0.64(-4)	32(-2)
0	8 8	-0.25(-4)	68(-3)	2	1 4	-0.805(-3)	17	3	6 7	0.46(-4)	88(-2)
0	10 10	-0.19(-4)	40(-2)	2	3 4	0.766(-3)	18	3	7 7	-0.30(-4)	56(-2)
				2	2 2	0.738(-3)	19	3	5 7	-0.30(-4)	35(-2)
1	2 3	0.007 116	78(+1)	2	1 1	0.658(-3)	25(-1)	3	1 7	0.26(-4)	21(-2)
1	1 3	0.006 319	38(+1)	2	3 5	-0.521(-3)	15	3	3 7	0.25(-4)	19(-2)
1	1 2	0.005 630	32(+1)	2	4 5	-0.509(-3)	19				
1	3 3	0.003 211	15(+1)	2	4 4	0.385(-3)	70(-1)	4	1 2	0.258(-3)	61(-2)
1	2 2	-0.001 138	22	2	1 5	0.364(-3)	69(-1)	4	2 2	0.224(-3)	50(-2)
1	2 4	0.001 021	24	2	2 5	-0.334(-3)	75(-1)	4	3 4	-0.112(-3)	24(-1)
1	3 5	-0.877(-3)	25	2	5 6	0.177(-3)	47(-1)	4	1 1	0.106(-3)	92(-3)
1	1 5	-0.755(-3)	16	2	3 6	-0.109(-3)	13(-1)	4	3 3	-0.79(-4)	75(-2)
1	1 1	0.640(-3)	19(-1)	2	1 6	0.69(-4)	49(-2)	4	4 4	-0.49(-4)	62(-2)
1	4 4	-0.561(-3)	94(-1)	2	6 6	-0.66(-4)	89(-2)	4	5 5	-0.36(-4)	71(-2)
1	2 5	-0.530(-3)	96(-1)	2	7 7	-0.54(-4)	12(-1)	4	4 5	0.35(-4)	50(-2)
1	1 4	0.462(-3)	37(-1)	2	6 7	0.47(-4)	70(-2)	4	3 5	-0.31(-4)	32(-2)
1	4 5	-0.443(-3)	81(-1)	2	5 7	0.27(-4)	19(-2)				
1	5 6	0.231(-3)	36(-1)	2	8 8	-0.19(-4)	48(-2)	5	2 2	-0.54(-4)	52(-2)
1	5 5	-0.228(-3)	27(-1)					5	3 3	-0.44(-4)	81(-2)
1	4 6	0.180(-3)	18(-1)	3	2 4	-0.663(-3)	43	5	2 3	-0.37(-4)	42(-2)
1	2 6	0.154(-3)	12(-1)	3	4 5	0.527(-3)	41	6	1 1	-0.46(-4)	68(-2)

TABLE 8. INTERSHELL EXCITATIONS  $^3S(1s2s) \rightarrow ^3S(\ell_a \ell_b)$

$\ell$	a b	EIGENVEC	ENERGY	$\ell$	a b	EIGENVEC	ENERGY	$\ell$	a b	EIGENVEC	ENERGY
0	3 4	0.001 325	22	1	2 6	0.295(-3)	44(-1)	2	3 5	-0.71(-4)	28(-2)
0	4 5	-0.966(-3)	22	1	3 5	0.281(-3)	26(-1)	2	5 7	-0.54(-4)	75(-2)
0	5 6	0.350(-3)	50(-1)	1	6 7	-0.124(-3)	20(-1)	2	4 7	0.45(-4)	48(-2)
0	3 6	0.304(-3)	27(-1)	1	1 7	0.116(-3)	12(-1)	2	3 7	0.37(-4)	31(-2)
0	4 7	0.297(-3)	49(-1)	1	4 7	-0.115(-3)	14(-1)	2	6 7	-0.23(-4)	17(-2)
0	3 5	-0.194(-3)	64(-2)	1	3 7	0.113(-3)	12(-1)				
0	6 7	0.174(-3)	22(-1)	1	5 7	-0.80(-4)	73(-2)	3	3 4	-0.330(-3)	84(-1)
0	4 9	-0.90(-4)	36(-2)	1	4 6	0.62(-4)	22(-2)	3	3 5	-0.325(-3)	94(-1)
0	5 8	0.77(-4)	42(-2)	1	6 8	-0.46(-4)	47(-2)	3	1 5	-0.317(-3)	83(-1)
0	6 9	-0.70(-4)	30(-2)	1	4 8	-0.38(-4)	27(-2)	3	1 2	0.307(-3)	31(-1)
0	7 8	-0.55(-4)	31(-2)	1	7 8	-0.27(-4)	19(-2)	3	1 4	-0.297(-3)	63(-1)
0	4 8	0.47(-4)	15(-2)					3	2 3	-0.275(-3)	29(-1)
				2	1 2	-0.001 668	54	3	4 5	-0.206(-3)	63(-1)
1	1 2	0.0101455	11(+2)	2	2 3	-0.001 646	64	3	2 5	0.179(-3)	35(-1)
1	2 3	-0.007 641	91(+1)	2	3 4	0.001 151	40	3	1 6	0.156(-3)	28(-1)
1	1 4	0.003 252	18(+1)	2	1 4	-0.001 048	29	3	3 6	0.145(-3)	25(-1)
1	3 4	0.003 208	23(+1)	2	1 3	-0.647(-3)	41(-1)	3	4 6	0.140(-3)	35(-1)
1	1 3	0.002 344	52	2	4 5	0.538(-3)	21	3	2 4	0.119(-3)	14(-1)
1	2 5	0.001 136	44	2	2 5	0.468(-3)	15	3	5 6	0.102(-3)	20(-1)
1	2 4	0.001 129	30	2	2 4	-0.448(-3)	82(-1)	3	2 6	-0.91(-4)	12(-1)
1	4 5	0.856(-3)	30	2	1 5	0.269(-3)	38(-1)	3	5 7	0.31(-4)	38(-2)
1	3 6	0.683(-3)	23	2	4 6	0.221(-3)	60(-1)	3	6 7	-0.22(-4)	21(-2)
1	1 6	0.468(-3)	96(-1)	2	5 6	-0.144(-3)	31(-1)				
1	1 5	-0.360(-3)	36(-1)	2	3 6	0.111(-3)	13(-1)	4	2 3	0.37(-4)	86(-3)
1	5 6	-0.344(-3)	80(-1)	2	2 6	0.111(-3)	14(-1)	4	3 4	0.35(-4)	23(-2)

See pages 296-297 for Explanation of Tables



TABLE 11. QUADRUPLE EXCITATIONS  $1s(\ell_a \ell_b)1s(\ell'_c \ell'_d)$ 

$\ell \ell'$	a b c d	EIGENVEC	ENERGY	$\ell \ell'$	a b c d	EIGENVEC	ENERGY
0 0	3 3 4 4	0.821(-3)	16	0 2	4 4 1 1	0.288(-3)	20(-1)
0 0	3 3 5 5	0.109(-3)	40(-2)	0 2	3 3 2 2	0.285(-3)	32(-1)
0 0	3 3 6 6	0.64(-4)	24(-2)	0 2	3 4 1 1	0.262(-3)	13(-1)
0 0	3 3 5 6	0.55(-4)	14(-2)	0 2	3 3 1 1	0.149(-3)	28(-2)
				0 2	3 3 3 3	0.96(-4)	19(-2)
0 1	4 4 1 1	0.004 729	52(+1)	0 2	3 3 4 4	0.96(-4)	49(-2)
0 1	3 4 1 1	0.004 641	37(+1)	0 2	3 4 2 2	-0.70(-4)	23(-2)
0 1	3 3 1 1	0.002 714	85	0 2	3 3 5 5	0.57(-4)	34(-2)
0 1	3 3 2 2	0.001 178	31				
0 1	5 5 1 1	0.611(-3)	12	1 2	1 1 2 2	0.002 005	16(+1)
0 1	5 6 1 1	0.523(-3)	13	1 2	2 2 1 1	0.518(-3)	59(-1)
0 1	3 3 1 2	0.464(-3)	35(-1)	1 2	1 1 2 3	-0.471(-3)	64(-1)
0 1	4 5 1 1	-0.454(-3)	59(-1)	1 2	1 1 4 4	0.439(-3)	10
0 1	6 6 1 1	0.374(-3)	81(-1)	1 2	1 1 3 4	0.337(-3)	41(-1)
0 1	3 4 2 2	-0.324(-3)	31(-1)	1 2	1 1 4 5	0.307(-3)	74(-1)
0 1	3 5 1 1	0.269(-3)	16(-1)	1 2	1 1 5 5	0.305(-3)	96(-1)
0 1	3 6 1 1	0.230(-3)	18(-1)	1 2	1 1 6 6	0.188(-3)	72(-1)
0 1	3 3 3 3	0.178(-3)	65(-2)	1 2	1 1 3 3	0.181(-3)	65(-2)
0 1	7 7 1 1	0.162(-3)	25(-1)	1 2	1 1 1 2	-0.169(-3)	70(-2)
0 1	3 3 1 3	0.142(-3)	32(-2)	1 2	1 1 2 4	-0.151(-3)	10(-1)
0 1	3 3 3 4	0.138(-3)	54(-2)	1 2	1 2 1 1	0.140(-3)	32(-2)
0 1	6 7 1 1	0.132(-3)	13(-1)	1 2	3 4 1 1	0.92(-4)	24(-2)
0 1	3 3 4 4	0.128(-3)	59(-2)	1 2	1 1 7 7	0.90(-4)	35(-1)
0 1	3 4 3 4	-0.87(-4)	26(-2)	1 2	1 1 2 5	0.79(-4)	45(-2)
0 1	3 3 5 5	0.87(-4)	43(-2)	1 2	2 2 3 3	0.77(-4)	18(-2)
0 1	7 8 1 1	-0.86(-4)	79(-2)	1 2	1 1 5 6	-0.77(-4)	91(-2)
0 1	4 4 2 2	0.86(-4)	27(-2)	1 2	1 1 1 4	-0.67(-4)	14(-2)
0 1	3 3 1 4	0.80(-4)	15(-2)	1 2	4 4 1 1	0.62(-4)	14(-2)
0 1	8 8 1 1	0.74(-4)	63(-2)	1 2	1 1 4 6	0.54(-4)	37(-2)
0 1	4 6 1 1	-0.69(-4)	19(-2)	1 2	1 1 8 8	0.25(-4)	85(-2)
0 1	3 3 4 5	0.68(-4)	22(-2)				
0 1	3 4 1 4	0.67(-4)	13(-2)	2 2	1 1 2 2	0.125(-3)	62(-2)
0 1	4 5 2 2	0.65(-4)	17(-2)				
0 1	3 7 1 1	-0.62(-4)	20(-2)	0 3	3 3 2 2	0.88(-4)	51(-2)
0 1	8 9 1 1	-0.61(-4)	35(-2)	0 3	3 3 2 3	-0.50(-4)	11(-2)
0 1	4 7 1 1	0.60(-4)	21(-2)	0 3	3 3 4 4	0.43(-4)	26(-2)
0 1	3 3 6 6	0.58(-4)	29(-2)				
0 1	5 5 2 2	0.49(-4)	11(-2)	1 3	1 1 2 2	0.663(-3)	28
0 1	9 9 1 1	0.46(-4)	16(-2)	1 3	1 1 2 3	-0.368(-3)	59(-1)
0 1	1010 1 1	0.25(-4)	67(-2)	1 3	1 1 4 4	0.320(-3)	14
				1 3	2 2 1 1	0.193(-3)	86(-2)
1 1	1 1 2 2	0.008 758	16(+2)	1 3	1 1 5 5	0.160(-3)	42(-1)
1 1	1 1 1 2	0.002 152	71	1 3	1 1 3 3	0.120(-3)	34(-2)
1 1	1 1 3 4	0.001 014	28	1 3	1 1 6 6	0.104(-3)	24(-1)
1 1	1 1 3 3	0.807(-3)	13	1 3	1 1 7 7	0.54(-4)	18(-1)
1 1	1 1 4 4	0.782(-3)	21				
1 1	1 1 2 3	-0.620(-3)	78(-1)	2 3	1 1 2 2	0.44(-4)	13(-2)
1 1	1 1 1 1	0.606(-3)	40(-1)				
1 1	1 1 4 5	0.593(-3)	16	0 4	3 3 3 3	0.46(-4)	26(-2)
1 1	1 1 2 4	-0.419(-3)	49(-1)				
1 1	1 1 5 5	0.419(-3)	99(-1)	1 4	1 1 3 3	0.343(-3)	15
1 1	1 1 3 5	0.355(-3)	48(-1)	1 4	1 1 4 4	0.152(-3)	60(-1)
1 1	1 1 5 6	-0.297(-3)	64(-1)	1 4	1 1 5 5	0.66(-4)	24(-1)
1 1	1 1 6 6	0.252(-3)	56(-1)				
1 1	1 1 1 3	0.239(-3)	88(-2)	1 5	1 1 2 2	0.182(-3)	60(-1)
1 1	1 1 1 4	0.206(-3)	96(-2)	1 5	1 1 3 3	0.82(-4)	29(-1)
1 1	1 1 7 7	0.173(-3)	55(-1)				
1 1	1 1 2 5	0.118(-3)	53(-2)	1 6	1 1 1 1	0.95(-4)	29(-1)
1 1	1 1 6 7	-0.110(-3)	17(-1)				
1 1	2 2 3 3	0.104(-3)	34(-2)				
1 1	2 2 3 4	-0.100(-3)	39(-2)				
1 1	1 1 3 6	0.95(-4)	48(-2)				
1 1	1 1 8 8	0.86(-4)	26(-1)				
1 1	1 1 4 6	-0.84(-4)	43(-2)				
1 1	1 1 4 7	-0.57(-4)	36(-2)				
1 1	2 2 4 4	0.57(-4)	15(-2)				
1 1	1 1 1 5	0.55(-4)	10(-2)				
1 1	1 1 2 6	-0.54(-4)	16(-2)				
1 1	1 1 9 9	0.40(-4)	91(-2)				
1 1	1 1 7 8	-0.24(-4)	15(-2)				

See pages 296-297 for Explanation of Tables