Oscillator strengths for S-P and P-D transitions for singly excited states of two-electron ions via Z-dependent perturbation theory

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(Received 19 September 1988)

Oscillator strengths for electric dipole transitions between singly excited S, P, and D states are calculated via Z-dependent perturbation theory. The transition matrix elements through first order are obtained from variational perturbation first-order wave functions. Second-order expansion coefficients for the matrix elements are then estimated with the aid of several approximants. These matrix elements, together with accurate transition energies, yield oscillator strengths for transitions between all S-P and P-D transitions between states of two-electron ions with principal quantum number up to 9 and for values of the nuclear charge up to approximately 30.

I. INTRODUCTION

Oscillator strengths of high accuracy for two-electron atoms have been available for many electric dipole transitions of the neutral atom[1] and several transitions of the isoelectronic sequence from nonrelativistic, variational calculations.[2] Relativistic calculations for a few transitions between lower-lying states have also been obtained via the random-phase approximation.[3] More recently, a large number of S-P and P-D transitions have been accurately computed for helium and some members of the isoelectronic sequence,[4] also by the use of nonrelativistic variational wave functions.

In the present paper, Z-dependent perturbation theory is applied to obtain oscillator strengths for the S-P and P-D allowed transitions between singly excited states of two-electron atoms. Relativistic transition energies for these states obtained in earlier papers of this series[5] are combined with the dipole-length transition matrix elements calculated here to yield the desired oscillator strengths. The calculated oscillator strengths are compared with other theoretical oscillator strengths where these are available. Only representative values are presented here, as the entire set of data would comprise over 7000 transitions for $Z \leq 30$. Nevertheless, any nontabulated oscillator strength can be easily computed from the data presented here.

II. METHOD

A. Z-dependent perturbation theory

In Z-dependent perturbation theory, the nonrelativistic Hamiltonian for an N-electron atom is given, in charge-scaled atomic units, by

$$H = H_0 + \frac{1}{Z} H_1 \ , \tag{1}$$

where the zero-order Hamiltonian is

$$H_0 = \sum_{l=1}^{2} \left[-\tfrac{1}{2}\nabla_i^2 - \frac{1}{r_i} \right] , \tag{2}$$

and the perturbation is

$$H_1 = \frac{1}{r_{12}} \ . \tag{3}$$

The nonrelativistic wave function for the state α is then given by

$$\Psi^{(\alpha)} = \sum_{n=0}^{\infty} Z^{-n} \psi_n^{(\alpha)} \ , \tag{4}$$

from which it follows that the transition matrix element is also given as a power series in Z^{-1},

$$M^{(\alpha,\beta)} = \langle \Psi^{(\alpha)} | Q | \Psi^{(\beta)} \rangle = \sum_n Z^{-(n+1)} M_n^{(\alpha,\beta)} \ , \tag{5}$$

where

$$M_n^{(\alpha,\beta)} = \sum_{m+l=n} \langle \psi_m^{(\alpha)} | Q | \psi_l^{(\beta)} \rangle \ , \tag{6}$$

and where $Q = r_1 \cos\theta_1 + r_2 \cos\theta_2$ is the appropriate opera-

tor for the length form of the oscillator strength. This matrix element is then combined with relativistic transition energies, also obtained from Z-dependent calculations[5] to yield the oscillator strength

$$f=\gamma(\alpha,\beta)(E^{(\alpha)}-E^{(\beta)})|M^{(\alpha,\beta)}|^2 , \quad (7)$$

with $\gamma(\alpha,\beta)=2$ or $\frac{5}{3}$ for S-P or P-D transitions, respectively. In this work we have made the usual assumption that the major portion of the relativistic correction to the oscillator strength is contained in the transition energy and not in the matrix element.

The zero-order matrix element is given by

TABLE I. Expansion coefficients for the transition matrix elements.

Transition		Singlets		Triplets		Transition		Singlets	Triplets
	M_0	M_1[a]	M_2[b]	M_1[a]	M_2[b]		M_0	M_1[a]	M_1[a]
2P-1S	1.053 50	−0.163 29	−0.382 06			6P-1S	0.126 67	0.075 79	
		(−0.163 27)				6P-2S	0.311 98	0.216 40	0.125 56
2P-2S	−3.000 00	−3.047 86	−3.206 79	−2.277 25	−2.098 42	6P-3S	0.785 32	0.475 72	0.277 98
		(−3.047 86)		(−2.277 24)		6P-4S	1.994 46	0.976 38	0.437 54
2P-3S	0.541 79	1.370 95	1.657 61	1.316 79	1.988 47	6P-5S	7.051 67	1.182 12	−1.066 59
		(1.370 95)		(1.316 78)		6P-6S	−30.740 84	−31.034 91	−28.669 43
2P-4S	0.220 72	0.523 43	0.546 55	0.476 58	0.682 56	6P-7S	6.274 66	12.639 93	14.273 81
		(0.523 45)		(0.476 57)		6P-8S	2.371 58	5.475 07	5.108 73
2P-5S	0.131 65	0.307 71	0.307 10	0.273 81	0.370 23	6P-9S	1.358 80	2.069 21	2.348 88
2P-6S	0.091 34	0.212 25		0.186 58		7P-1S	0.099 14	0.061 38	
2P-7S	0.068 71	0.159 23		0.138 87		7P-2S	0.235 57	0.168 66	0.102 52
2P-8S	0.054 36	0.125 81		0.109 09		7P-3S	0.549 31	0.360 04	0.229 02
2P-9S	0.044 52	0.102 96		0.088 89		7P-4S	1.190 42	0.660 03	0.413 38
3P-1S	0.421 88	0.154 16	−0.204 92			7P-5S	2.811 63	1.451 26	0.593 50
		(0.154 00)				7P-6S	9.560 19	1.307 09	−1.499 87
3P-2S	1.769 47	0.556 56	−0.161 60	−0.292 31	−1.098 32	7P-7S	−42.000 00	−42.261 76	−39.570 08
		(0.556 56)		(−0.292 32)		7P-8S	8.647 73	16.408 37	19.403 47
3P-3S	−7.348 47	−7.497 50	−7.357 40	−6.315 76	−5.722 91	7P-9S	3.236 59	8.984 27	7.329 28
		(−7.497 43)		(−6.315 71)		8P-1S	0.080 42	0.050 87	
3P-4S	1.410 77	3.169 80	4.300 90	3.341 49	5.049 98	8P-2S	0.186 83	0.136 56	0.084 83
		(3.169 84)		(3.341 49)		8P-3S	0.416 31	0.285 12	0.188 75
3P-5S	0.559 80	1.144 20	1.170 13	1.170 63	1.353 10	8P-4S	0.829 71	0.507 92	0.342 90
3P-6S	0.330 40	0.655 12		0.663 50		8P-5S	1.662 48	0.811 96	0.558 54
3P-7S	0.228 51	0.447 94		0.450 52		8P-6S	3.756 88	2.303 87	0.773 51
3P-8S	0.171 96	0.335 13		0.335 41		8P-7S	12.443 67	1.210 93	−2.021 65
3P-9S	0.136 34	0.264 83		0.264 05		8P-8S	−54.990 91	−55.195 37	−52.188 61
4P-1S	0.248 69	0.125 85	−0.098 40			8P-9S	11.396 46	21.000 58	25.161 85
		(0.125 85)				9P-1S	0.066 99	0.043 39	
4P-2S	0.740 32	0.426 27	0.180 51	0.161 62	−0.490 71	9P-2S	0.153 27	0.114 31	0.072 48
		(0.426 01)		(0.161 61)		9P-3S	0.331 64	0.235 45	0.159 20
4P-3S	3.157 72	0.755 64	−0.440 83	−0.453 05	−2.001 60	9P-4S	0.628 27	0.412 39	0.286 43
		(0.755 98)		(−0.453 05)		9P-5S	1.152 74	0.624 37	0.469 59
4P-4S	−13.416 41	−13.628 66	−12.733 03	−12.042 75	−10.369 09	9P-6S	2.201 86	0.848 97	0.707 77
		(−13.628 71)		(−12.042 74)		9P-7S	4.830 62	3.695 95	1.034 59
4P-5S	2.655 97	5.720 40	8.161 87	6.190 01	8.919 14	9P-8S	15.702 28	0.788 47	−2.612 38
4P-6S	1.032 45	2.007 58		2.114 61		9P-9S	−69.713 70	−69.509 02	−66.314 32
4P-7S	0.602 57	1.118 11		1.176 80					
4P-8S	0.414 34	0.759 74		0.794 18					
4P-9S	0.310 97	0.567 68		0.589 99					
5P-1S	0.170 41	0.096 46	−0.059 95						
5P-2S	0.446 84	0.292 95	0.257 03	0.153 58	−0.107 25				
5P-3S	1.304 57	0.678 26	0.144 54	0.295 97	−0.572 99				
5P-4S	4.917 77	0.973 91	−0.984 73	−0.716 36	−3.451 78				
5P-5S	−21.213 20	−21.479 92	−19.522 28	−19.493 15	−16.787 68				
5P-6S	4.277 35	9.000 28		9.865 39					
5P-7S	1.636 69	3.143 54		3.314 40					
5P-8S	0.945 76	1.652 90		1.800 18					
5P-9S	0.646 35	1.120 70		1.211 58					

[a] For M_1, the first entry is from the present variational perturbation calculations. The entries in parentheses are essentially exact results of Ref. 7.

[b] Values of M_2 obtained by differencing the results of Refs. 2 and 4.

$$M_0^{NL,N'L'} = 4 A_{NL} A_{N'L'} \frac{2L'(2L+4)!}{(2L+1)(2L'+1)} \left[\frac{NN'}{N+N'} \right]^{2L+5}$$

$$\times F_2 \left[2L+5 | L+1-N, L'+1-N' | 2L+2, 2L'+2 | \frac{2N'}{N+N'}, \frac{2N}{N+N'} \right], \tag{8a}$$

TABLE II. Expansion coefficients for the matrix elements.

Transition		Singlets		Triplets	
	M_0	M_1[a]	M_2[b]	M_1[a]	M_2[b]
2*P*-3*D*	2.451 85	2.701 73	2.816 55	1.598 29	1.866 98
		(2.689 26)		(1.597 09)	
2*P*-4*D*	0.882 89	0.860 14	0.880 89	0.814 20	0.703 32
		(0.849 78)		(0.813 41)	
2*P*-5*D*	0.503 53	0.467 02	0.411 17	0.510 08	0.449 57
2*P*-6*D*	0.341 76	0.309 04		0.361 00	
2*P*-7*D*	0.253 87	0.226 42		0.274 44	
2*P*-8*D*	0.199 28	0.176 62		0.218 50	
2*P*-9*D*	0.162 36	0.145 13		0.179 72	
3*P*-3*D*	−5.196 15	−5.196 15	−5.206 17	−5.386 86	−5.391 08
		(−5.121 68)		(−5.386 41)	
3*P*-4*D*	3.906 76	4.445 29	4.678 19	2.142 59	2.383 39
		(4.449 59)		(2.142 77)	
3*P*-5*D*	1.532 83	1.620 65	1.593 61	1.222 12	1.040 80
3*P*-6*D*	0.899 09	0.922 56		0.796 19	
3*P*-7*D*	0.619 50	0.627 09		0.576 41	
3*P*-8*D*	0.465 06	0.467 84		0.444 96	
3*P*-9*D*	0.368 11	0.371 12		0.358 48	
4*P*-3*D*	0.672 48	0.446 14	0.261 36	1.443 42	1.488 02
		(0.444 00)		(1.443 74)	
4*P*-4*D*	−10.733 13	−10.649 74	−9.455 71	−10.992 02	−11.527 38
		(−10.652 37)		(−10.991 84)	
4*P*-5*D*	5.700 49	6.542 98	7.598 73	2.810 59	3.230 33
4*P*-6*D*	2.265 16	2.445 95		1.661 02	
4*P*-7*D*	1.335 35	1.394 31		1.091 27	
4*P*-8*D*	0.923 30	0.957 90		0.798 37	
4*P*-9*D*	0.695 33	0.722 81		0.621 27	
5*P*-3*D*	0.249 32	0.178 79	0.075 64	0.500 60	0.498 24
5*P*-4*D*	1.572 60	1.097 79	0.853 29	3.181 71	3.437 49
5*P*-5*D*	−17.748 25	−17.656 95	−30.922 46	−18.068 65	−17.591 64
5*P*-6*D*	7.831 42	9.021 19		3.581 49	
5*P*-7*D*	3.100 79	3.421 95		2.154 16	
5*P*-8*D*	1.823 66	1.879 66		1.397 65	
5*P*-9*D*	1.259 55	1.310 34		1.033 47	
6*P*-3*D*	0.142 16	0.109 05		0.280 14	
6*P*-4*D*	0.579 86	0.537 52		1.089 04	
6*P*-5*D*	2.802 48	2.007 91		5.481 23	
6*P*-6*D*	−26.290 68	−26.168 08		−26.669 13	
6*P*-7*D*	10.298 92	11.623 31		4.382 71	
6*P*-8*D*	4.046 07	5.372 04		2.991 01	
6*P*-9*D*	2.368 08	2.108 77		1.514 67	
7*P*-3*D*	0.096 37	0.057 31		0.189 07	
7*P*-4*D*	0.328 71	0.202 55		0.602 31	
7*P*-5*D*	1.027 09	1.040 78		1.860 68	
7*P*-6*D*	4.366 04	3.009 46		8.330 70	
7*P*-7*D*	−36.373 06	−36.173 71		−36.800 37	
7*P*-8*D*	13.102 71	14.157 33		5.195 70	
7*P*-9*D*	5.103 61	8.363 37		4.054 97	
8*P*-3*D*	0.071 60	0.053 60		0.140 13	
8*P*-4*D*	0.222 00	0.129 11		0.404 66	
8*P*-5*D*	0.578 77	0.327 30		1.002 63	

TABLE II. (*Continued*).

Transition	Singlets		Triplets	
	M_0	M_1[a] M_2[b]	M_1[a]	M_2[b]
8*P*-6*D*	1.591 23	2.139 49	2.966 26	
8*P*-7*D*	6.264 38	4.036 03	11.668 40	
8*P*-8*D*	−48.000 00	−47.622 89	−48.456 67	
8*P*-9*D*	16.242 61	17.182 30	5.943 54	
9*P*-3*D*	0.056 28	0.046 94	0.110 34	
9*P*-4*D*	0.164 63	0.101 98	0.300 09	
9*P*-5*D*	0.389 19	0.210 53	0.677 98	
9*P*-6*D*	0.891 81	0.365 51	1.305 67	
9*P*-7*D*	2.272 00	3.837 71	4.428 11	
9*P*-8*D*	8.497 93	4.321 68	15.398 94	
9*P*-9*D*	−61.173 52	−60.169 45	−61.515 90	

[a]For M_1, the first entry is from the present variational perturbation calculations. The entry in parentheses is the essentially exact result of Ref. 7.
[b]Values of M_2 obtained by differencing the results of Refs. 2 and 4.

where F_2 is Appell's hypergeometric function in two variables,[6] $L'=L+1$, and the A_{NL} are normalization constants for the zero-order wave functions,

$$A_{NL}=\left[\frac{(N+L)!(2L+1)}{2(N-L-1)!}\right]^{1/2}\frac{2^L}{N^{L+2}(2L+1)!}\ . \tag{8b}$$

The first-order matrix element has been calculated using the variational perturbation wave functions of Ref. 5. For almost all of the states considered here, only first-order matrix elements have been directly calculated. Thus M_1 is based on the accurate two-electron ψ_1 calculated there. Tables I and II list the M_0 and M_1 for the states considered here.

B. The transition matrix elements

Laughlin[7] made use of a generalization of the screening approximation of Dalgarno and Stewart[8] to improve the convergence of the first-order transition matrix element. When the transitions involve a change in the principal quantum number, the matrix element is written as

$$M=\frac{M_0}{Z_\sigma}+\frac{m_1}{Z_\sigma^2}\ , \tag{9}$$

where $m_1=M_1-\sigma M_0$ and $Z_\sigma=Z-\sigma$. Laughlin chose σ so as to give the Hartree-Fock expansion of M correct through terms in Z^{-3}. However, for transitions in which the principal quantum number does not change, the approximation of Dalgarno and Stewart[8] was found to be more accurate where, with $s=M_1/M_0$,

$$M=\frac{M_0}{Z-s}\ . \tag{10}$$

In the present paper this screening approximation is extended by an additional term,

$$M=\frac{M_0}{Z_\sigma}+\frac{m_1}{Z_\sigma^2}+\frac{m_2}{Z_\sigma^3}\ , \tag{11}$$

which, with m_1 and Z_σ as above and $m_2=M_2-2\sigma M_1+\sigma^2 M_0$, also gives the matrix element correct to terms in Z^{-3}. Equation (9) can also be modified slightly so that it takes the form of Padé approximants

$$M=\frac{M_0+(M_1-\sigma_1 M_0)/Z}{Z-\sigma_1}\ , \tag{12a}$$

a [1/1] Padé approximant, or

$$M=M_0/[Z-\sigma_1+(\sigma_1^2-\sigma_2)/Z]\ , \tag{12b}$$

a [0/2] Padé approximant. Then $\sigma_1=M_2/M_1$ and $\sigma_2=M_2/M_0$ yield Z expansions of M correct through terms in Z^{-3}. All these approximants were found to represent M more accurately than Eq. (9), even for transitions in which the principle quantum number does not change. However, the screening approximation of Eq. (11) proved more useful in most cases than the Padé ap-

TABLE III. Higher-order expansion coefficients of the matrix elements M_n for two transitions.[a]

n	$2\,^1P$-$1\,^1S$	$2\,^3P$-$2\,^3S$
0	1.053 50	−3.000 00
1	−0.163 27	−2.277 24
2	−0.384 18	−2.056 38
3	−0.196 83	−1.884 82
4	−0.033 36	−1.671 95
5	−0.008 91	−1.400 30
6	−0.210 85	−1.087 03
7	−0.186 83	−0.766 68
8	−0.041 65	−0.302 43
9	0.038 53	
10	−0.013 06	
11	−0.076 70	
12	−0.030 96	

[a]Obtained from the results of Ref. 9.

TABLE IV. Comparison of differenced M_2 with approximate $\tilde{M}_2$ of Eq. (13).

Transition	M_2	$\tilde{M}_2$	N-M	α	σ
		Singlets			
2*P*-1*S*	−0.382	0.150	1		
3*P*-1*S*	−0.205	−0.142	2		
4*P*-1*S*	−0.098	−0.116	3	$-0.92M_1$	0.28
5*P*-1*S*	−0.060	−0.089	4		
2*P*-2*S*	−3.207	−2.895	0		
3*P*-3*S*	−7.357	−7.123	0		
4*P*-4*S*	−12.733	−12.947	0	$0.95M_1$	0.78
5*P*-5*S*	−19.522	−20.406	0		
3*P*-2*S*	−0.162	−0.230	1		
4*P*-3*S*	−0.441	−0.576	1	$0.35(M_1+\Delta)$	0.60
5*P*-4*S*	−0.985	−1.039	1		
4*P*-2*S*	0.181	0.071	2		
5*P*-3*S*	0.145	0.033	2	$0.64(M_1+\Delta)$	0.53
5*P*-2*S*	0.257	0.089	3		
2*P*-3*S*	1.658	1.837	−1		
3*P*-4*S*	4.301	4.248	−1	$1.34M_1$	0.85
4*P*-5*S*	8.162	7.665	−1		
2*P*-4*S*	0.547	0.586	−2		
3*P*-5*S*	1.170	1.282	−2	$1.12M_1$	0.68
2*P*-5*S*	0.307	0.345	−3		
		Triplets			
2*P*-2*S*	−2.098	−2.050	0		
3*P*-3*S*	−5.723	−5.684	0		
4*P*-4*S*	−10.369	−10.838	0	$0.90M_1$	0.59
5*P*-5*S*	−16.788	−17.544	0		
3*P*-2*S*	−1.098	−1.295	1		
4*P*-3*S*	−2.002	−2.235	1	$0.55(M_1+\Delta)$	0.72
5*P*-4*S*	−3.452	−3.493	1		
4*P*-2*S*	−0.491	−0.304	2		
5*P*-3*S*	−0.573	−0.520	2	$0.73(M_1+\Delta)$	0.74
5*P*-2*S*	−0.107	−0.102	3		
2*P*-3*S*	1.988	2.080	−1		
3*P*-4*S*	5.050	5.144	−1	$0.65M_1^2/M_0$	0.86
4*P*-5*S*	8.919	9.377	−1		
2*P*-4*S*	0.683	0.669	−2		
3*P*-5*S*	1.353	1.591	−2	$0.65M_1^2/M_0$	1.01
2*P*-5*S*	0.370	0.370	−3		
		Singlets			
3*P*-3*D*	−5.206	−5.070	0		
4*P*-4*D*	−9.456	−10.546	0	$0.99M_1$	1.12
5*P*-5*D*	−30.922	−17.480	0		
4*P*-3*D*	0.261	0.408	1	$0.92M_1$	0.95
5*P*-4*D*	0.853	1.010	1		
5*P*-3*D*	0.076	0.151	2	$M_1+0.40\Delta$	1.05
2*P*-3*D*	2.817	2.716	−1		
3*P*-4*D*	4.678	4.494	−1	$1.01M_1$	0.55
4*P*-5*D*	7.599	6.608	−1		
2*P*-4*D*	0.881	0.858	−2		
3*P*-5*D*	1.594	1.637	−2	$1.01M_1$	0.95
2*P*-5*D*	0.411	0.472	−3		

TABLE IV. (*Continued*).

Transition	M_2	$\tilde{M}_2$	N-M	α	σ
		Triplets			
3*P*-3*D*	−5.391	−5.377	0		
4*P*-4*D*	−11.527	−10.979	0	$M_1-0.05\Delta$	0.85
5*P*-5*D*	−17.592	−18.053	0		
4*P*-3*D*	1.488	1.516	1	$1.05M_1$	0.80
5*P*-4*D*	3.437	3.341	1		
5*P*-3*D*	0.498	0.493	2	$M_1-0.03\Delta$	0.38
2*P*-3*D*	1.867	1.821	−1		
3*P*-4*D*	2.383	2.443	−1	$1.14M_1$	0.69
4*P*-5*D*	3.230	3.204	−1		
2*P*-4*D*	0.703	0.797	−2		
3*P*-5*D*	1.041	1.198	−2	$0.98M_1$	0.80
2*P*-5*D*	0.450	0.500	−3		

TABLE V. Oscillator strengths for $M\,^1S$–$N\,^1P$ transitions for various Z. In each case, the first entry is the result of the present paper while the second entry, if present, is the variational result of Refs. 2 and 4.

M	N	2	3	4	5	6	7	8	9
					$Z=2$				
1		0.277 74	0.081 48	0.029 87	0.014 36	0.008 03	0.004 96	0.003 28	0.002 29
		0.276 16	0.073 44	0.029 863	0.015 039	0.008 628	0.005 405	0.003 610	0.002 530
2		0.376 33	0.150 84	0.049 69	0.022 65	0.012 28	0.007 45	0.004 87	0.003 39
		0.376 44	0.151 34	0.049 16	0.022 34	0.012 13	0.007 360	0.004 813	0.003 325
3		0.149 34	0.626 85	0.144 81	0.050 45	0.024 29	0.013 87	0.008 73	0.005 94
		0.145 47	0.626 2	0.143 90	0.050 5	0.024 19	0.013 68	0.008 57	0.005 76
4		0.024 88	0.299 79	0.855 97	0.150 41	0.053 30	0.025 26	0.014 90	0.009 75
		0.025 87	0.3075	0.858	0.1463	0.052 8	0.025 88	0.014 95	0.009 54
5		0.009 88	0.049 72	0.462 65	1.077 99	0.159 12	0.061 94	0.025 05	0.014 86
		0.009 652	0.055 48	0.476	1.083	0.1526	0.055 6	0.027 60	0.016 13
6		0.005 02	0.019 92	0.077 23	0.629 84	1.296 16	0.167 48	0.080 35	0.022 65
		0.004 769	0.021 11	0.0862	0.647	1.305	0.1609	0.0588	0.0293
7		0.002 93	0.010 31	0.030 77	0.107 47	0.772 12	1.511 17	0.172 97	0.110 86
		0.002 739	0.010 64	0.033 05	0.117 2	0.819	1.53	0.1705	0.0623
8		0.001 87	0.006 12	0.016 12	0.040 77	0.176 31	0.884 06	1.725 09	0.175 22
		0.001 730	0.006 23	0.016 81	0.0451	0.1482	0.993	1.745	0.181
9		0.001 27	0.003 97	0.009 71	0.021 62	0.045 40	0.278 93	1.015 00	1.932 01
		0.001 167	0.003 999	0.009 94	0.023 05	0.0571	0.1793	1.166	1.963
					$Z=3$				
1		0.456 91	0.115 60	0.043 74	0.021 30	0.012 01	0.007 45	0.004 94	0.003 45
		0.4566	0.1106	0.0437	0.0217				
2		0.211 55	0.255 14	0.071 95	0.031 15	0.016 52	0.009 89	0.006 41	0.004 43
		0.2126	0.257 07	0.073	0.031				
3		0.099 91	0.362 69	0.261 86	0.078 59	0.035 68	0.019 71	0.012 17	0.008 14
		0.0947	0.3624	0.2651	0.080				
4		0.019 23	0.207 16	0.500 60	0.281 47	0.086 56	0.039 10	0.022 07	0.014 03
		0.0188	0.205	0.500	0.285				
5		0.007 61	0.040 19	0.324 06	0.632 66	0.307 89	0.098 88	0.041 09	0.023 41
		0.0072	0.0413	0.322	0.63				

TABLE V. (*Continued*).

M	N	2	3	4	5	6	7	8	9
					$Z=3$				
6		0.003 87	0.016 11	0.063 63	0.447 79	0.814 38	0.328 02	0.117 20	0.040 92
7		0.002 26	0.008 33	0.025 39	0.089 03	0.543 24	0.955 07	0.340 51	0.145 94
8		0.001 44	0.004 95	0.013 27	0.034 20	0.137 65	0.627 50	0.798 85	0.358 04
9		0.000 98	0.003 21	0.007 99	0.018 08	0.039 12	0.208 05	0.751 52	0.941 27
					$Z=5$				
1		0.608 93	0.137 43	0.051 96	0.025 31	0.014 26	0.008 84	0.005 87	0.004 10
		0.608 91	0.135 4	0.052 0	0.025 5				
2		0.113 96	0.332 75	0.086 48	0.036 40	0.019 07	0.011 33	0.007 32	0.005 03
		0.114 36	0.333 71	0.087 1	0.037				
3		0.070 56	0.198 06	0.355 43	0.098 15	0.043 22	0.023 47	0.014 36	0.009 52
		0.068 54	0.198 1	0.357 09	0.098 7				
4		0.014 72	0.152 86	0.275 24	0.389 97	0.110 56	0.048 83	0.027 03	0.016 89
		0.014 43	0.152 0	0.275	0.391 7				
5		0.005 83	0.032 35	0.242 95	0.349 61	0.436 22	0.125 78	0.053 45	0.029 77
		0.005 65	0.032 6	0.242	0.35				
6		0.002 97	0.013 06	0.052 33	0.342 88	0.428 56	0.467 52	0.143 77	0.055 84
7		0.001 73	0.006 76	0.021 08	0.073 95	0.422 45	0.501 57	0.503 28	0.168 85
8		0.001 11	0.004 02	0.011 04	0.029 07	0.108 01	0.499 58	0.548 82	0.537 75
9		0.000 75	0.002 61	0.006 64	0.015 36	0.034 71	0.154 05	0.585 46	0.618 50
					$Z=10$				
1		0.722 62	0.149 68	0.055 94	0.027 12	0.015 26	0.009 45	0.006 26	0.004 37
		0.722 63	0.149 2	0.056 0	0.027 2				
2		0.053 36	0.385 97	0.095 40	0.039 49	0.020 61	0.012 19	0.007 85	0.005 37
		0.053 430	0.386 24	0.095 6	0.039 6				
3		0.053 86	0.092 97	0.422 14	0.110 58	0.048 30	0.025 93	0.015 76	0.010 39
		0.053 390	0.092 98	0.422 55	0.110 7				
4		0.011 72	0.121 65	0.129 51	0.468 95	0.129 01	0.056 02	0.030 56	0.018 88
		0.011 65	0.121 47	0.129 5	0.469 4				
5		0.004 65	0.027 02	0.196 20	0.164 89	0.565 49	0.148 75	0.063 44	0.034 77
		0.004 61	0.027 1	0.196 1	0.165				
6		0.002 38	0.011 08	0.045 49	0.298 93	0.205 36	0.572 63	0.159 35	0.065 92
7		0.001 39	0.005 75	0.018 44	0.065 77	0.349 37	0.240 79	0.623 67	0.180 42
8		0.000 89	0.003 42	0.009 66	0.026 26	0.086 95	0.420 90	0.279 43	0.674 60
9		0.000 60	0.002 22	0.005 81	0.013 83	0.031 46	0.116 55	0.496 39	0.314 81

proximants, due in large measure to the availability of σ as a free parameter to further optimize the approximant.

The problem, then, is to obtain reasonable estimates for M_2 in order to be able to construct the above approximants. The M_2 are apparently available in the literature[9] for only two of the transitions considered here, $2\,^3P-2\,^3S$ and $2\,^1P-1\,^1S$. Estimates of these coefficients can also be extracted, via a differencing procedure, from variationally calculated f values that extend over a sufficiently wide range of Z values. These can then serve to test the various possible approximants to M_2 that will actually be utilized in the present calculations. Results obtained via this differencing procedure are also presented in Tables I and II for those transitions for which sufficient data are available. To obtain the values of M_2 shown there, the corresponding variationally calculated, nonrelativistic transition energies were used to extract the transition matrix elements from the theoretical f values of Refs. 2 and 4. The known values of M_0 and M_1 were then used to eliminate their contribution to the matrix element, leaving M_2 as the leading term to be obtained by differencing.

From Tables I and II, it is clear that the expansion coefficients for the matrix element can vary widely in magnitude from one transition to another. However, there is surprisingly little variation among the M_n for a particular transition. In fact, one can see that the ratio M_2/M_1 is roughly 1 for many of these transitions. More careful examination shows that the ratios and/or the differences of successive coefficients are very nearly constant over a range of transitions. Examination of these

M_n in the two cases where they have actually been computed to higher order, suggests why this might be so. Table III lists these coefficients from Ref. 9. The slight oscillation of the triplet expansion coefficients makes extrapolation a reasonable possibility, while the stronger oscillation of the singlet coefficients is more problematic but, in this instance at least, extrapolation yields reasonable values for M_2.

Thus it appears that the M_2 can be estimated more reliably via the M_0 and M_1 corresponding to that particular transition than from examining trends along a sequence of transitions. With this in mind a variety of approximants for M_2 were examined. The most reliable of these took the form

$$\tilde{M}_2=\alpha M_1 , \tag{13a}$$

$$\frac{\tilde{M}_2}{M_1}=\alpha\frac{M_1}{M_0} , \tag{13b}$$

$$\tilde{M}_2=\alpha(M_1+\Delta) , \tag{13c}$$

or

$$\tilde{M}_2=M_1+\alpha\Delta , \tag{13d}$$

where $\Delta=M_1-M_0$. The parameter α can be determined from the M_2 of Tables I and II. From the data in these tables, it is clear that these separate roughly into three groups depending upon whether, in the transition, the principal quantum number increases, decreases, or remains the same. It also is clear that further improvement could be expected by considering each group of transitions with $\delta=N-M$ separately, but this approach would result in considerable complication of the method, while the data for larger δ are too limited (or nonexistent) to make this possible. However, considerable improvement is obtained by also considering the two cases $\delta=\pm1$ separately, and this has been done throughout. Sets of (α,σ) were thus obtained for these five groups of transitions by minimizing the rms deviation (weighted by Z) of the present f values with respect to the accurate, variationally calculated f values of Refs. 2 and 4 over the range of values of Z available there. Thus the fits for these parameters are limited to values of the principal quantum number less than or equal to 5. A greater range of transitions could have been incorporated into the fitting procedure by using $Z=2$ data alone, but it was felt that relying solely on the data for such a low value of Z would tend to overcorrect the approximate $\tilde{M}_2$ for higher-order contributions to the matrix element. This, in turn, would yield poorer results for intermediate to large values of Z where the present method is most useful. Optimum (α,σ) values were obtained for each of the approximants of Eqs. (13) and the best approximant was selected. This was done separately for the singlet and triplet *MS-NP* and *MP-ND* transitions with $N<M-1$, $N=M-1$, $N=M$, $N=M+1$, and $N>M+1$; a total of 20 separate groups of transitions (actually 21, since the $1\,^1S$-$N\,^1P$ transitions were also separately optimized). For each group of transitions the approximant, together with the α and σ producing the smallest Z-weighted rms deviation for the f values, was selected. The values of α thus obtained are generally quite close to those values which minimize the rms deviation between the $\tilde{M}_2$ yielded by Eqs. (13) and the M_2 of Tables I and II, obtained by differencing available f values. Inspection of the M_2 of Tables I and II indicates that some of these M_2 are rather crudely estimated. The α of Eqs. (13) were therefore obtained by optimizing on the f values instead. The final optimum set of approximants utilized in these calculations is presented in Table IV.

III. RESULTS AND DISCUSSION

Only a sampling of the final results that can be generated with the data available here can be presented. The data of Tables I, II, and IV permit calculation of all *MS-NP* and *MP-ND* transitions up to $N, M=9$; a total of 248 possible transitions for any one value of Z. In these tables, the values of M_0 are exact, but the M_1 are approximate, coming as they do from variationally calculated first-order wave functions. The accuracy to be expected of these first-order matrix elements can be seen in Tables I and II where they are compared, where possible, to the essentially exact values of Ref. 7. The M_1 computed here are of sufficient precision to produce accurate f values.

Tables V–VIII present f values for representative transitions for values of Z ranging from 2 to 10 for which accurate, variationally calculated values are available for comparison. The latter are all nonrelativistic calculations. Hence, for those transitions only, the present values are obtained using the same transition energies as were used in the earlier, variational calculations. Thus the differences between the present and earlier results are entirely due to differences in the computed matrix elements. The remaining transitions in these tables are calculated using the relativistic transition energies of Ref. 5. In any case, within the accuracy of these calculations and for these low values of Z, the difference produced in the oscillator strengths by using relativistic or nonrelativistic energies is not significant.

The calculations for the singlet S-P transitions show that for $Z=3$, the percent relative difference between the present results and the variationally calculated f values is always less than 6%, with all but 5 of the 20 transitions compared having errors under 2%. For $Z=5$ the largest relative difference is about 3% with all but 5 under 1%. By $Z=10$ all relative differences are under 1% with all but 3 under 0.3%. Typically the worst agreement is obtained for those transitions where the S state is more highly excited than the P state. For the triplet S-P transitions, this situation is reversed, with the worst agreement occurring for those transitions where the P state is the most highly excited. The largest relative difference for $Z=3$ in this case is less than 1.5% for all transitions but two, whose relative differences are about 7% and 3.5%. For $Z=5$, all relative differences are under 2%

TABLE VI. Oscillator strengths for $M\,^3S-N\,^3P$ transitions for various Z. In each case, the first entry is the result of the present paper while the second entry, if present, is the variational result Refs. 2 and 4.

M	N	2	3	4	5	6	7	8	9
					$Z=2$				
2		0.538 67	0.046 84	0.021 64	0.012 48	0.007 40	0.004 69	0.003 13	0.002 23
		0.539 086	0.064 461	0.025 769	0.012 491	0.006 982	0.004 299	0.002 836	0.001 970
3		0.209 88	0.893 44	0.049 94	0.023 29	0.013 96	0.008 61	0.005 64	0.003 91
		0.208 53	0.890 9	0.050 08	0.022 92	0.011 99	0.007 07	0.004 54	0.003 09
4		0.032 65	0.434 15	1.216 99	0.052 77	0.024 60	0.015 09	0.009 54	0.006 43
		0.031 72	.4357	1.215 3	0.044 23	0.021 63	0.011 78	0.007 16	0.004 71
5		0.011 35	0.067 33	0.653 92	1.531 08	0.056 08	0.026 04	0.016 03	0.010 39
		0.011 34	0.067 61	0.668	1.531	0.041 5	0.021 11	0.011 74	0.007 27
6		0.005 40	0.023 89	0.100 39	0.871 53	1.840 83	0.059 76	0.027 79	0.016 76
		0.005 488	0.024 70	0.104 0	0.903	1.842	0.0403	0.0210	0.011 8
7		0.003 03	0.011 66	0.035 23	0.133 85	1.063 24	2.148 01	0.063 55	0.030 92
		0.003 113	0.012 21	0.038 2	0.140 3	1.139	2.151	0.039 9	0.021 2
8		0.001 88	0.006 69	0.017 43	0.044 81	0.223 23	1.237 17	2.453 37	0.067 72
		0.001 949	0.007 07	0.019 10	0.051 7	0.176	1.376	2.458	0.040 0
9		0.001 26	0.004 24	0.010 15	0.022 68	0.040 29	0.338 91	1.382 67	2.750 25
		0.001 306	0.004 51	0.011 17	0.026 0	0.065 0	0.212	1.613	2.764
					$Z=3$				
2		0.307 93	0.174 09	0.055 55	0.025 65	0.013 97	0.008 48	0.005 53	0.003 84
		0.307 940	0.187 1	0.057 5	0.026				
3		0.117 16	0.513 54	0.185 00	0.061 54	0.029 64	0.016 73	0.010 45	0.007 02
		0.117 10	0.512 8	0.186 86	0.061 4				
4		0.021 59	0.255 02	0.703 92	0.200 45	0.067 52	0.033 12	0.019 05	0.012 13
		0.021 47	0.255 0	0.703 6	0.196 2				
5		0.008 06	0.048 17	0.397 16	0.889 42	0.218 99	0.073 76	0.036 29	0.021 12
		0.008 06	0.048 0	0.400	0.890				
6		0.003 98	0.018 45	0.075 80	0.543 56	1.072 72	0.238 00	0.079 97	0.038 92
7		0.002 28	0.009 33	0.029 08	0.104 25	0.677 29	1.295 28	0.257 08	0.087 04
8		0.001 44	0.005 46	0.014 87	0.039 20	0.150 82	0.790 30	1.634 24	0.276 52
9		0.000 97	0.003 51	0.008 83	0.020 38	0.043 22	0.204 54	0.909 15	1.500 97
					$Z=5$				
2		0.162 62	0.285 67	0.078 37	0.033 77	0.017 87	0.010 67	0.006 90	0.004 75
		0.162 6	0.291 2	0.079	0.033 7				
3		0.075 47	0.271 89	0.308 91	0.089 08	0.040 10	0.021 93	0.013 46	0.008 94
		0.075 438	0.271 71	0.310 29	0.089 10				
4		0.015 23	0.170 36	0.373 97	0.339 98	0.100 07	0.045 69	0.025 42	0.015 87
		0.015 22	0.170 14	0.373 9	0.339 02				
5		0.005 87	0.035 38	0.271 41	0.473 63	0.380 78	0.111 10	0.050 96	0.028 65
		0.005 87	0.035 3	0.271 7	0.473 6				
6		0.002 95	0.014 01	0.057 41	0.382 40	0.574 27	0.411 25	0.120 60	0.055 31
7		0.001 70	0.007 19	0.022 82	0.080 44	0.477 39	0.676 38	0.448 42	0.132 12
8		0.001 08	0.004 25	0.011 84	0.031 75	0.109 54	0.576 73	0.788 05	0.486 65
9		0.000 73	0.002 74	0.007 08	0.016 64	0.037 77	0.142 12	0.673 95	0.850 76
					$Z=10$				
2		0.074 20	0.364 03	0.091 95	0.038 38	0.020 10	0.011 91	0.007 67	0.005 25
		0.074 20	0.365 5	0.092 1	0.038 3				
3		0.055 13	0.124 27	0.399 58	0.106 44	0.046 86	0.025 22	0.015 34	0.010 12
		0.055 116	0.124 25	0.400 05	0.106 46				

TABLE VI. (*Continued*).

M	N	2	3	4	5	6	7	8	9
4		0.011 76	0.127 67	0.171 26	0.444 36	0.123 92	0.054 53	0.029 79	0.018 40
		0.011 764	0.127 59	0.171 3	0.444 25				
5		0.004 62	0.028 03	0.206 53	0.217 18	0.535 44	0.141 23	0.062 25	0.034 25
		0.004 617	0.028 0	0.206 5	0.217 17				
6		0.002 34	0.011 42	0.047 35	0.314 55	0.269 90	0.544 83	0.147 81	0.065 85
7		0.001 36	0.005 90	0.019 12	0.068 21	0.370 70	0.316 48	0.596 57	0.162 04
8		0.000 87	0.003 50	0.009 98	0.027 42	0.086 29	0.452 77	0.365 04	0.650 03
9		0.000 59	0.002 27	0.005 98	0.014 39	0.032 98	0.109 01	0.534 58	0.409 07

TABLE VII. Oscillator strengths for $N\,{}^1P$-$M\,{}^1D$ transitions for various Z. In each case, the first entry is the result of the present paper while the second entry, if present, is the variational result of Ref. 4.

M	N	2	3	4	5	6	7	8	9
					$Z=2$				
3		0.706 40	0.021 16	0.015 33	0.003 12	0.001 22	0.000 55	0.000 35	0.000 24
		0.710 16	0.021 14	0.015 31	0.003 11	0.001 188	0.000 594	0.000 345	0.000 220
4		0.121 06	0.650 82	0.039 74	0.039 04	0.009 37	0.003 00	0.001 49	0.000 90
		0.120 26	0.648 1	0.040 1	0.039 3	0.008 38	0.003 27	0.001 664	0.000 979
5		0.043 74	0.142 10	0.646 13	0.061 32	0.067 65	0.017 47	0.005 21	0.002 63
		0.043 26	0.141 3	0.648	0.059 73	0.068 4	0.015 01	0.005 95	0.003 06
6		0.021 20	0.056 93	0.152 65	0.665 73	0.072 40	0.098 53	0.031 23	0.007 04
		0.020 95	0.056 29	0.152 9	0.670	0.074	0.100 8	0.022 6	0.009 03
7		0.012 05	0.029 33	0.063 82	0.162 56	0.680 65	0.088 08	0.130 91	0.050 31
		0.011 90	0.028 90	0.063 6	0.163 2	0.703	0.089	0.135	0.030 7
8		0.007 57	0.017 38	0.033 95	0.068 74	0.182 35	0.685 94	0.101 60	0.162 18
		0.007 464	0.017 08	0.033 6	0.069 3	0.173 2	0.741	0.105	0.171
9		0.005 11	0.011 27	0.020 63	0.037 34	0.070 64	0.208 60	0.708 60	0.115 49
		0.005 015	0.011 04	0.020 34	0.037 3	0.074 5	0.183 7	0.784	0.120
					$Z=3$				
3		0.714 80	0.024 30	0.014 89	0.003 03	0.001 20	0.000 52	0.000 34	0.000 23
		0.711 61	0.024 32	0.015 01	0.003 06				
4		0.117 75	0.654 06	0.043 93	0.038 53	0.009 34	0.002 89	0.001 42	0.000 86
		0.119 27	0.651 72	0.043 97	0.038 78				
5		0.042 17	0.142 13	0.649 24	0.061 54	0.067 90	0.017 53	0.004 96	0.002 49
		0.042 732	0.141 41	0.651 1	0.061 62				
6		0.020 33	0.056 56	0.154 10	0.673 52	0.098 93	0.096 61	0.031 65	0.006 51
7		0.011 51	0.029 02	0.063 74	0.165 04	0.678 17	0.134 03	0.123 26	0.052 26
8		0.007 22	0.017 15	0.033 79	0.068 25	0.192 23	0.683 43	0.039 98	0.146 41
9		0.004 88	0.011 14	0.020 57	0.037 28	0.067 24	0.237 60	0.753 37	0.188 00
					$Z=5$				
3		0.706 99	0.017 84	0.016 04	0.003 27	0.001 27	0.000 59	0.000 37	0.000 24
		0.706 33	0.017 83	0.015 95	0.003 249				
4		0.118 38	0.641 53	0.030 94	0.041 22	0.009 52	0.003 22	0.001 61	0.000 96
		0.119 31	0.642 04	0.030 92	0.041 07				
5		0.042 62	0.140 90	0.635 60	0.042 53	0.073 01	0.017 57	0.005 67	0.002 87
		0.042 873	0.140 73	0.638 3	0.042 51				
6		0.020 63	0.056 39	0.152 82	0.666 01	0.053 05	0.103 68	0.029 55	0.007 85
7		0.011 71	0.029 00	0.063 55	0.164 00	0.675 35	0.061 13	0.135 76	0.045 57
8		0.007 35	0.017 17	0.033 75	0.068 59	0.185 68	0.695 58	0.065 25	0.162 63
9		0.004 96	0.011 14	0.020 50	0.037 26	0.068 78	0.218 72	0.730 70	0.055 34

TABLE VII. (*Continued*).

M	*N*	2	3	4	5	6	7	8	9
					$Z=7$				
3		0.703 19	0.013 30	0.016 66	0.003 38	0.001 32	0.000 62	0.000 38	0.000 25
		0.703 13	0.013 29	0.016 570	0.003 365				
4		0.119 13	0.635 03	0.022 58	0.042 63	0.009 67	0.003 41	0.001 71	0.001 02
		0.119 68	0.635 70	0.022 57	0.042 50				
5		0.043 03	0.140 38	0.628 39	0.030 74	0.076 96	0.017 77	0.006 08	0.003 08
		0.043 129	0.140 31	0.630 3	0.030 72				
6		0.020 90	0.056 52	0.153 05	0.672 35	0.036 67	0.107 36	0.028 40	0.008 51
7		0.011 88	0.029 10	0.063 76	0.164 82	0.669 44	0.042 42	0.141 47	0.042 27
8		0.007 46	0.017 23	0.033 86	0.069 24	0.180 41	0.693 67	0.047 76	0.171 76
9		0.005 03	0.011 17	0.020 55	0.037 51	0.069 67	0.206 71	0.727 62	0.050 16

TABLE VIII. Oscillator strengths for $N\,^3P$-$M\,^3D$ transitions for various Z. In each case, the first entry is the result of the present paper while the second entry, if present, is the variational result of Ref. 4.

M	*N*	2	3	4	5	6	7	8	9
					$Z=2$				
3		0.605 77	0.111 65	0.037 23	0.006 90	0.002 59	0.001 29	0.000 75	0.000 48
		0.610 22	0.112 1	0.037 0	0.006 90	0.002 58	0.001 284	0.000 743	0.000 474
4		0.121 31	0.474 18	0.200 47	0.087 89	0.016 73	0.006 38	0.003 23	0.001 90
		0.122 85	0.447 6	0.200 9	0.088 3	0.017 0	0.006 50	0.003 27	0.001 919
5		0.046 69	0.124 99	0.434 74	0.279 74	0.145 72	0.028 28	0.010 69	0.005 54
		0.047 01	0.124 6	0.439	0.280 1	0.147 0	0.028 9	0.011 16	0.005 67
6		0.023 34	0.053 20	0.126 00	0.425 03	0.354 68	0.207 22	0.043 51	0.013 24
		0.023 47	0.053 01	0.124 0	0.430	0.354	0.210	0.042 0	0.016 27
7		0.013 50	0.028 24	0.055 92	0.128 69	0.424 94	0.425 98	0.269 52	0.062 07
		0.013 56	0.028 16	0.055 2	0.125 4	0.434	0.426	0.276	0.055 5
8		0.008 57	0.017 02	0.030 66	0.057 86	0.140 05	0.429 59	0.496 02	0.330 02
		0.008 603	0.016 98	0.030 3	0.057 1	0.128	0.445	0.496	0.343
9		0.005 80	0.011 14	0.018 94	0.032 42	0.055 88	0.153 62	0.434 63	0.564 16
		0.005 823	0.011 12	0.018 71	0.031 8	0.058 9	0.132	0.460	0.564
					$Z=3$				
3		0.623 62	0.091 03	0.032 98	0.006 20	0.002 33	0.001 17	0.000 68	0.000 43
		0.624 65	0.090 76	0.032 78	0.006 20				
4		0.123 56	0.505 33	0.161 07	0.078 57	0.015 35	0.005 89	0.002 98	0.001 75
		0.123 21	0.503 4	0.160 59	0.078 72				
5		0.047 23	0.128 79	0.473 32	0.223 39	0.131 54	0.026 30	0.010 03	0.005 17
		0.046 796	0.127 84	0.470 6	0.222 66				
6		0.023 55	0.054 48	0.130 99	0.471 57	0.285 21	0.187 52	0.039 98	0.012 94
7		0.013 59	0.028 83	0.057 74	0.134 59	0.475 99	0.313 31	0.244 10	0.055 76
8		0.008 61	0.017 33	0.031 48	0.059 94	0.144 49	0.476 38	0.219 91	0.300 77
9		0.005 83	0.011 34	0.019 44	0.033 54	0.058 78	0.158 22	0.498 60	0.684 64
					$Z=5$				
3		0.648 85	0.057 88	0.027 09	0.005 23	0.001 98	0.000 99	0.000 57	0.000 37
		0.649 26	0.057 78	0.027 05	0.005 227				
4		0.123 54	0.545 01	0.101 66	0.065 73	0.013 29	0.005 12	0.002 59	0.001 53
		0.123 21	0.543 76	0.101 50	0.065 87				
5		0.046 42	0.132 94	0.521 17	0.140 61	0.112 83	0.023 10	0.008 90	0.004 59
		0.046 157	0.132 43	0.519 4	0.140 38				

TABLE VIII. (*Continued*).

M	*N*	2	3	4	5	6	7	8	9
					$Z=5$				
6		0.022 98	0.055 38	0.138 26	0.533 47	0.178 15	0.159 35	0.034 57	0.012 05
7		0.013 21	0.029 06	0.059 89	0.144 16	0.537 84	0.212 33	0.209 36	0.048 02
8		0.008 35	0.017 39	0.032 39	0.063 39	0.152 93	0.555 45	0.233 38	0.259 66
9		0.005 64	0.011 33	0.019 85	0.034 95	0.063 55	0.164 89	0.577 54	0.302 72
					$Z=7$				
3		0.661 56	0.041 73	0.024 47	0.004 78	0.001 82	0.000 91	0.000 53	0.000 34
		0.661 80	0.041 69	0.024 46	0.004 778				
4		0.123 21	0.564 72	0.073 11	0.059 99	0.012 38	0.004 77	0.002 42	0.001 42
		0.123 00	0.564 00	0.073 05	0.060 08				
5		0.045 90	0.134 77	0.544 84	0.101 04	0.105 88	0.021 78	0.008 42	0.004 32
		0.045 746	0.134 48	0.543 8	0.100 95				
6		0.022 66	0.055 85	0.142 48	0.572 98	0.128 96	0.146 88	0.032 01	0.011 55
7		0.012 99	0.029 17	0.061 13	0.150 23	0.568 44	0.154 61	0.193 79	0.044 19
8		0.008 20	0.017 41	0.032 89	0.065 45	0.156 60	0.590 65	0.177 53	0.241 36
9		0.005 54	0.011 33	0.020 09	0.035 84	0.065 91	0.167 81	0.616 32	0.210 13

TABLE IX. Oscillator strengths for NP-MS transitions for $Z=26$. In each case, the first entry is the result of the present paper while the second entry, if present, is the RRPA result of Ref. 3.

M	*N*	2	3	4	5	6	7	8	9
					Singlets				
1		0.798 12	0.156 70	0.057 91	0.027 94	0.015 66	0.009 68	0.006 41	0.004 46
		0.706 2	0.137 7	0.050 7	0.024 4				
2		0.031 56	0.422 46	0.101 30	0.041 52	0.021 46	0.012 66	0.008 14	0.005 56
		0.032	0.364	0.088	0.036				
3		0.045 53	0.055 58	0.467 28	0.118 48	0.050 55	0.027 00	0.016 35	0.010 75
		0.043	0.056	0.400	0.103				
4		0.010 12	0.105 88	0.077 76	0.521 98	0.134 63	0.058 31	0.031 65	0.019 48
		0.009 3	0.101	0.078	0.446				
5		0.004 03	0.024 13	0.172 38	0.099 24	0.580 85	0.151 08	0.065 41	0.035 79
		0.003 7	0.023	0.164	0.099				
6		0.002 05	0.009 82	0.039 76	0.241 76	0.120 35	0.641 54	0.168 35	0.071 97
7		0.001 20	0.005 11	0.016 34	0.056 25	0.311 38	0.141 30	0.701 76	0.186 72
8		0.000 77	0.003 04	0.008 59	0.023 10	0.075 28	0.379 46	0.173 46	0.765 14
9		0.000 52	0.001 98	0.005 18	0.012 24	0.029 66	0.096 19	0.450 63	0.195 69
					Triplets				
2		0.040 47	0.414 94	0.100 19	0.041 17	0.021 31	0.012 57	0.008 08	0.005 52
		0.035	0.367	0.089	0.036				
3		0.045 81	0.069 04	0.459 22	0.117 05	0.050 07	0.026 76	0.016 21	0.010 66
		0.042	0.049	0.404	0.103				
4		0.010 10	0.107 69	0.095 71	0.513 06	0.132 90	0.057 81	0.031 39	0.019 31
		0.009 2	0.098	0.068	0.450				
5		0.004 01	0.024 43	0.175 59	0.121 71	0.571 10	0.148 50	0.065 04	0.035 63
		0.003 7	0.022	0.160	0.086				
6		0.002 03	0.009 92	0.040 33	0.246 37	0.147 19	0.631 35	0.163 99	0.072 00
7		0.001 19	0.005 15	0.016 56	0.056 97	0.318 35	0.172 81	0.692 06	0.179 73
8		0.000 76	0.003 07	0.008 70	0.023 48	0.074 81	0.390 42	0.202 29	0.755 99
9		0.000 52	0.001 99	0.005 24	0.012 43	0.030 23	0.093 14	0.463 90	0.228 08

while, for $Z=10$, all are less than 0.5%. For the *P-D* transitions the percent relative differences for the singlet and triplet states, respectively, are less than 1.5% and 1% for $Z=3$, less than 1% and 0.6% for $Z=5$, and less than 0.6% and 0.3% for $Z=7$.

The accuracy to be expected for those transitions where one or more principal quantum number is greater than 5 (for which accurate comparison data are not available for $Z \geq 3$) can be estimated by examining the tables for $Z=2$. Here, accurate variationally computed oscillator strengths up to principal quantum number equal to 9 are available.[4] Except for one or two anomalous points, the present calculations for $Z=2$ are in fairly good agreement with the variationally calculated f values throughout this range of transitions, although the agreement is somewhat worse for those transitions where the *P* state is more highly excited. This is most noticeable for the triplet *S-P* transitions; somewhat less so for the singlet *P-D* transitions. Thus, no deterioration of the accuracy of the oscillator strengths for $Z \geq 3$ and principal quantum number greater than 5 is expected.

For large *Z* values, relatively few accurate f values are available for comparison. Table IX compares a few relativistic f values computed via the relativistic random-phase approximation (RRPA),[3] with f values computed here using relativistic transition energies[5] and our approximate transition matrix elements. These are for *S-P* transitions only. Examination of Table IX, where data for $Z=26$ are compared, indicates that the present calculation agrees with the RRPA results to at least one significant figure, typically giving percentage differences of around 5% to 15%. Since the comparison data are given to only two or three significant figures, it is difficult to assess the accuracy of the present calculations.

IV. SUMMARY

The data in Tables I–IV allow computation of the electric dipole-length matrix elements for the transitions considered here through second-order in perturbation theory. These include all singly excited states of two-electron atoms with principal quantum number up to 9 and values of the nuclear charge up to approximately 30. Accurate relativistic transition energies are then combined with these matrix elements to yield the oscillator strengths.

The results of Tables V–IX show that the present method is capable of providing results of reasonable accuracy with a minimum of computational effort for a very large number of transitions.

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