Radiative lifetimes of the bound excited states of magnesium and beryllium

T. N. Chang
Department of Physics, University of Southern California, Los Angeles, California 90089-0484
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We present the radiative lifetimes for series of bound excited states of neutral magnesium and beryllium derived from the transition probabilities calculated in a simple configuration-interaction procedure using a finite basis set constructed from B splines. Our calculated radiative lifetimes compare very well with the most accurate recent state-selected excitation measurements. In particular, our calculation has removed the discrepancy between earlier theoretical and experimental lifetimes for the first few Mg I $3snd\ ^1D$ states that are strongly affected by the configuration mixing from $3pp$ configuration series.

I. INTRODUCTION

By populating the upper level of an atom with state-selected multiphoton excitation, the radiative lifetime τ of the excited state can be determined without the cascading correction required in a more conventional approach involving collisional excitations such as in a beam-foil experiment commonly employed for *atomic ions* of various positive charged states. The reduction of the experimental uncertainty due to the absence of cascading effect in such experiment has led to a much closer agreement between observed lifetimes from different measurements. One such example is seen in a recent time-resolved fluorescence experiment in a vapor cell for the $3sns\ ^1S$ and $3snd\ ^1D$ series of Mg I by Chantepie *et al.*[1] Their measured lifetimes agree very well with earlier similar beam measurement by Jönsson *et al.*[2] and to a lesser extent with the delayed-coincidence measurement using pulsed discharge technique by Schaefer.[3] In addition, the radiative lifetimes have been measured for the Mg I $3sns\ ^3S$ and $3snd\ ^3D$ series following pulsed laser excitation from the metastable $3s3p\ ^3P$ Mg I beam populated by electron impact by Kwiatkowski, Teppner, and Zimmerman.[4] The laser-excitation technique has also been employed earlier to measure the absolute transition probability for the *weak* $3s^2\ ^1S \rightarrow 3s3p\ ^3P$ transition in Mg I and Si III.[5]

These state-selected excitation measurements, made possible by routine availability of a high intensity laser with wavelengths compatible with the excitation energies for *neutral atoms,* have provided the necessary experimental accuracy required for the establishment of the quantitative reliability of the theoretical transition probabilities. Once the quantitative reliability of any theoretical approach is established, it becomes straightforward to extend the theoretical calculation to atomic ions not strongly affected by the relativistic interactions along the isoelectronic sequence, for which the similar state-selected excitation measurements are not performed routinely due to the lack of lasers of shorter wavelengths needed for the excitations in multiply ionized atoms. The experimental uncertainty due to the cascading effect in a beam-foil experiment could be reduced significantly if the atomic transitions data involving upper levels are taken into account in the lifetime measurement.[6,7] A *reliable* theoretical estimation of the atomic transition probabilities for the higher excited states could, in principle, provide such data. In addition to the beam-foil experiment, which has been performed routinely for the lifetime measurements of low-lying excited states in atomic ions, the complementary electron capture technique,[8,9] involving collisions between multiply ionized atoms and neutral two-electron atoms such as helium gas, could be employed to populate the higher excited states of the resulting ions. The accuracy in lifetime and transition probability measurements in the collisional excitation experiments should improve with help from the cascading correction estimated either theoretically or experimentally.

For divalent atoms, such as alkaline-earth atoms and their associated isoelectronic sequences, some of the atomic transitions are dominated by the strong electron correlation.[1,10] For example, for the Mg I $3snd\ ^1D$ series, all existing experiments have shown that the lifetimes τ do not increase monotonically as a function of the effective quantum number n^* along the $3snd\ ^1D$ series.[1] Qualitatively, this n^* dependence is well understood and has been interpreted as the result of strong configuration mixing between the $3sd$ and $3pp$ configuration series.[1,10] Quantitatively, on the other hand, for the first few states in the Mg I $3snd\ ^1D$ series, which are dominated by strong configuration mixing, the theoretical lifetimes τ from the multiconfiguration Hartree-Fock[11] (MCHF) and model potential[12] calculations are either too large or too small in comparison with the observed values in spite of the general acceptance of the reliability of these two theoretical calculations.[1]

Theoretically, a reliable radiative lifetime calculation for states affected strongly by the configuration mixing usually requires elaborate numerical effort involving sophisticated optimum procedure. Extension of such a procedure to a large number of excited states is often hindered by the need of separate optimizations of the initial and final states of each transition included in the transi-

tion probability calculation. As a result, a large-scale calculation is often carried out with a theoretically less elaborate but computationally more efficient numerical procedure at the expense of quantitative reliability. In our recent attempt to examine systematically the *outer-shell* electron correlation of a divalent atom between two valence electrons outside a closed-shell ^1S core, we have demonstrated that a simple configuration-interaction (CI) procedure, with configurations represented by two-electron L^2 basis sets constructed from one-electron orbitals subject to a single-particle frozen-core Hartree-Fock (FCHF) potential, is capable of leading to highly reliable quantitative atomic data without the time-consuming *optimization* procedure.[10,13–15] By including the *continuum* contribution in a *quasicomplete* discrete basis set[14] of radial basis-set functions constructed from B splines confined in a finite radius R, our calculation has shown that the calculated energy levels and oscillator strengths of beryllium are at least comparable to and often superior to other more elaborate theoretical calculations.[14]

In this paper, we present the results of an application of this simple CI procedure to the transition probabilities for emissions from bound excited states of magnesium and beryllium. The theoretical radiative lifetimes derived from the calculated transition probabilities will be compared with other available theoretical and experimental data. In particular, we will show that our calculation has successfully removed the discrepancy between the existing calculations and experiments for the lifetimes of the Mg I $3snd\ ^1D$ series discussed earlier. The computational procedure of the simple CI calculation has been discussed in detail in our recent papers.[10,13–15] In Sec II, we briefly outline a few of the important elements in the calculation of the transition probabilities and the radiative lifetimes. In Sec. III, we present the results of an application of the simple CI calculation to the radiative lifetimes of Mg I and Be I. Some of the transition probabilities are tabulated to illustrate the theoretical uncertainty in radiative lifetimes due to the limited numerical accuracy in weak transitions of relatively small oscillator strengths.

II. CALCULATIONAL PROCEDURE

The radiative lifetime τ_i of an upper atomic level i is given by the simple expression

$$\frac{1}{\tau_i} = \sum_j A_{ij} \tag{1}$$

where A_{ij} is the transition probability for the emission from an upper state i to an allowed lower state j. The transition probability A_{ij} can be expressed in terms of the oscillator strength f_{ij}^e for *emission* and the energy difference ΔE_{ij} between states i and j by the relation[16]

$$A_{ij} = 8.0323(\Delta E_{ij})^2 f_{ij}^e \ . \tag{2}$$

The transition probability A_{ij} is given in units of ns^{-1} (i.e., $10^9\ sec^{-1}$) and the theoretical excitation energy ΔE_{ij} is given in Ry units in all our calculations.

The simple CI procedure employed in our energy and oscillator-strength calculations, with a finite basis set constructed from B splines, has been presented in detail elsewhere.[10,13–15] Our calculation has shown that the calculated excitation energies for most of the transitions between bound excited states of Mg I and Be I agree with the observed values to less than 10^{-3} Ry.[14] In addition to this close agreement in excitation energies, the quantitative accuracy of our calculated oscillator strength f is also demonstrated by (i) the close agreement between our calculated f values and the available experimental data,[14] (ii) the small fluctuation of the calculated oscillator strengths as the number of the configurations included in the state wave functions of the initial and final states of the transition is increased, and (iii) the closed agreement between the *converged* length and velocity f values. In the present calculation, the fluctuation of the converged f values is generally less than 1% and for the length approximation often less than 0.1%. The agreement between the length and velocity results is typically about 1–2 %, except for a few of the $^1S \rightarrow {}^1P$ transitions for which the difference could be as high as 5–6 % when the oscillator strengths are small. Because of the close agreement between the length and velocity results, only the *average* f values between the length and velocity calculations are used in the calculations of the transition probabilities and the radiative lifetimes reported in Sec. III. More extensive tabulations of the oscillator strengths for transitions in Mg I and Be I are given elsewhere.[15]

III. RESULTS AND DISCUSSIONS

In Table I, we compare the radiative lifetimes of the Mg I $3snd\ ^1D$ and $3sns\ ^1S$ series calculated in the simple CI procedure with other experimental and theoretical values. More extensive comparisons between earlier theoretical and experimental results can be found in Refs. 1 and 17. The agreement between the state-selected excitation measurements by Chantepie *et al.*[1] and Jönsson *et al.*[2] is very good. The measured lifetimes from the delayed-coincidence experiment with pulsed discharge excitation by Schaefer[3] are in satisfactory agreement with the state-selected experiments, except for the $3s3d\ ^1D$ and $3s5s\ ^1S$ states. The theoretical lifetimes between the MCHF calculation by Froese Fischer[11] and the more recent L^2 CI calculation by Moccia and Spizzo[17] are generally in close agreement, except for the $3s3d\ ^1D$ state for which the calculated lifetime would be longer than 100 ns if theoretical ΔE is used in the L^2 CI calculation. The lifetimes from the model potential calculation by Victor *et al.*[12] are in qualitative agreement with other theoretical values but deviate slightly from others for few of the states listed in Table I.

For $3s3d\ ^1D$ state, the close-coupling result by Mendoza and Zeippen[18] is in very good agreement with the results from the present simple CI calculation and the state-selected excitation measurements. The lifetimes from the MCHF and L^2 CI calculations are longer than the experimental data. As for the model potential calculation, its value is slightly below the values from the state-selected excitation measurements. For the $3s4d\ ^1D$ and $3s5d\ ^1D$ states, the lifetimes from MCHF and L^2 CI

TABLE I. Experimental and theoretical radiative lifetimes τ in ns for the excited ^1D and ^1S states of Mg I. Both length (L) and velocity (V) results from Moccia and Spizzo (Ref. 17) are listed.

Reference	τ(ns) for Mg I $3snl\ ^1L$ series					
	$3s3d\ ^1D$	$3s4d\ ^1D$	$3s5d\ ^1D$	$3s6d\ ^1D$	$3s7d\ ^1D$	$3s8d\ ^1D$
Chantepie *et al.*[a]	72±4	53±3	45±1	52±1	71±2	94±4
Jönsson *et al.*[b]	81±6	57±3	50±4	54±3	70±6	93±7
Schaefer[c]	57±4	55±1	44±2	50±2	73±2	85±11
Froese Fischer[d]	90	39	37	50	65	92
Victor, Stewart, and Laughlin[e]	67	57	47	63		
Moccia and Spizzo[f]—L	93[g]	42.3	37.9	47.6	64.6	90.4
Moccia and Spizzo[f]—V	93[g]	42.8	38.3	48.2	66.1	88.7
Mendoza and Zeippen[h]	78.8					
Present	79.5	52.4	42.6	51.8	69.2	94.1
	$3s4s\ ^1S$	$3s5s\ ^1S$	$3s6s\ ^1S$	$3s7s\ ^1S$	$3s8s\ ^1S$	
Chantepie *et al.*[a]	44±5	102±5	215±7	353±27	559±50	
Jönsson *et al.*[b]	47±3	100±5	211±12	350±16	548±35	
Schaefer[c]		163±8	201±4			
Froese Fischer[d]	45	102	204	367		
Victor, Stewart, and Laughlin[e]	41	95	178			
Moccia and Spizzo[f]—L	47.4	104	205	365	595	
Moccia and Spizzo[f]—V	48.2	106	209	370	599	
Mendoza and Zeippen[h]	45.1					
Saraph[i]	44	102	207	367		
Present	45.8	100	196	336	570	

[a]Reference 1.
[b]Reference 2.
[c]Reference 3.
[d]Reference 11.
[e]Reference 12.
[f]Reference 17.
[g]The experimental transition energy is employed.
[h]Reference 18.
[i]Reference 19.

calculations are slightly shorter than the observed values whereas the results from the model potential calculation as well as the present simple CI calculation are in close agreement with the experimental data. For the higher $3snd\ ^1D$ states, the agreement between the theoretical and experimental lifetimes is generally very good.

The difference in theoretical lifetimes for the $3s(3\text{-}5)d\ ^1D$ states can be attributed to the noticeable difference in the calculated oscillator strengths for the $3s3p\ ^1P \rightarrow 3snd\ ^1D$ transitions shown in Table V of Ref. 10. As we have pointed out earlier[10] that for the Mg I $3snd\ ^1D$ series, higher configuration series are required for a more satisfactory convergence in the state wave-function calculation. The MCHF, model potential, and the L^2 CI results should all improve if more configurations are included in the calculation. We also note that the lack of *continuum* contribution in our earlier *bound* only CI calculation[10] and the model potential calculation[12] does not affect noticeably the oscillator strengths for the $3s3p\ ^1P \rightarrow 3snd\ ^1D$ transitions.

For the Mg I $3sns\ ^1S$ series, all theoretical lifetimes listed in Table I appear to agree well with the experimental data. However, a closer examination of the theoretical calculation will show that for most of these states, the accuracy of the calculated radiative lifetime may be limited only to the first two digits. Table II shows that all of the $3sns\ ^1S \rightarrow 3smp\ ^1P$ transitions contribute significantly to the radiative decay from the upper $3sns\ ^1S$ states of Mg I. In particular, we note that in spite of the small oscillator strengths for the $3sns\ ^1S \rightarrow 3s3p\ ^1P$ emissions shown in Table III, its *branching ratios* B_{3p}, or equivalently, the *relative transition probability,* defined by

$$B_j = \frac{A_{ij}}{\sum_j A_{ij}} , \tag{3}$$

are comparable to the branching ratios from other emissions with much larger oscillator strengths. In fact, the oscillator strengths f listed in Table III for the $3sns\ ^1S \rightarrow 3s3p\ ^1P$ emissions from few selected theoretical calculations, with an accuracy limited to one to two digits for most of the transitions, are remarkably close for oscillator strengths as small as 10^{-4}. In spite of the close agreement in theoretical f values, the reliability of the theoretical radiative lifetime still suffers from the relatively large uncertainty in oscillator strength for emission with small f value but large radiative transition probabil-

TABLE II. Calculated transition probability A_{ij} in 10^7 sec^{-1} and branching ratio B_j in % for selected $^{1,3}S$ to $^{1,3}P$ emissions of Be I and Mg I.

Beryllium			Magnesium		
Transition $(i \rightarrow j)$	A_{ij}	$B_j(\%)$	Transition $(i \rightarrow j)$	A_{ij}	$B_j(\%)$
$2s6s\ ^1S \rightarrow 2s2p\ ^1P$	0.302	39.9	$3s7s\ ^1S \rightarrow 3s3p\ ^1P$	0.060	20.3
$2s6s\ ^1S \rightarrow 2s3p\ ^1P$	0.212	28.0	$3s7s\ ^1S \rightarrow 3s4p\ ^1P$	0.096	32.4
$2s6s\ ^1S \rightarrow 2s4p\ ^1P$	0.132	17.5	$3s7s\ ^1S \rightarrow 3s5p\ ^1P$	0.068	23.0
$2s6s\ ^1S \rightarrow 2s5p\ ^1P$	0.111	14.6	$3s7s\ ^1S \rightarrow 3s6p\ ^1P$	0.073	24.3
$2s5s\ ^1S \rightarrow 2s2p\ ^1P$	0.499	41.3	$3s6s\ ^1S \rightarrow 3s3p\ ^1P$	0.133	26.0
$2s5s\ ^1S \rightarrow 2s3p\ ^1P$	0.403	33.3	$3s6s\ ^1S \rightarrow 3s4p\ ^1P$	0.187	36.8
$2s5s\ ^1S \rightarrow 2s4p\ ^1P$	0.307	25.4	$3s6s\ ^1S \rightarrow 3s5p\ ^1P$	0.190	37.2
$2s4s\ ^1S \rightarrow 2s2p\ ^1P$	0.975	48.1	$3s5s\ ^1S \rightarrow 3s3p\ ^1P$	0.385	38.6
$2s4s\ ^1S \rightarrow 2s3p\ ^1P$	1.054	51.9	$3s5s\ ^1S \rightarrow 3s4p\ ^1P$	0.614	61.4
$2s3s\ ^1S \rightarrow 2s2p\ ^1P$	3.394	100.0	$3s4s\ ^1S \rightarrow 3s3p\ ^1P$	2.184	100.0
$2s6s\ ^3S \rightarrow 2s2p\ ^3P$	0.951	66.4	$3s7s\ ^3S \rightarrow 3s3p\ ^3P$	0.652	67.8
$2s6s\ ^3S \rightarrow 2s3p\ ^3P$	0.239	16.7	$3s7s\ ^3S \rightarrow 3s4p\ ^3P$	0.150	15.6
$2s6s\ ^3S \rightarrow 2s4p\ ^3P$	0.130	9.1	$3s7s\ ^3S \rightarrow 3s5p\ ^3P$	0.080	8.4
$2s6s\ ^3S \rightarrow 2s5p\ ^3P$	0.112	7.8	$3s7s\ ^3S \rightarrow 3s6p\ ^3P$	0.079	8.2
$2s5s\ ^3S \rightarrow 2s2p\ ^3P$	1.803	69.1	$3s6s\ ^3S \rightarrow 3s3p\ ^3P$	1.183	69.6
$2s5s\ ^3S \rightarrow 2s3p\ ^3P$	0.475	18.2	$3s6s\ ^3S \rightarrow 3s4p\ ^3P$	0.291	17.1
$2s5s\ ^3S \rightarrow 2s4p\ ^3P$	0.330	12.7	$3s6s\ ^3S \rightarrow 3s5p\ ^3P$	0.225	13.3
$2s4s\ ^3S \rightarrow 2s2p\ ^3P$	4.228	75.7	$3s5s\ ^3S \rightarrow 3s3p\ ^3P$	2.737	75.2
$2s4s\ ^3S \rightarrow 2s3p\ ^3P$	1.355	24.3	$3s5s\ ^3S \rightarrow 3s4p\ ^3P$	0.904	24.8
$2s3s\ ^3S \rightarrow 2s2p\ ^3P$	15.034	100.0	$3s4s\ ^3S \rightarrow 3s3p\ ^3P$	10.021	100.0

ity from an upper state. As a result, a detailed examination of the branching ratio for each of the allowed emissions is necessary before the accuracy of the theoretical lifetimes can be determined.

In Table IV, we compare the experimental lifetimes of the Mg I $3snd\ ^3D$ and $3sns\ ^3S$ series with the radiative lifetimes from few selected theoretical calculations. The agreement is generally very good with few exceptions. Again, we note that a theoretical uncertainty of 2–3 % in the calculated radiative lifetimes for the Mg I $3sns\ ^3S$ series could be introduced by the small oscillator strengths (see, e.g., Ref. 15) but large branching ratio for the $3sns\ ^3S \rightarrow 3s3p\ ^3P$ emissions shown in Table II.

The lifetime measurements for the excited states of Be I are mostly limited to the collisional excitation experiments. Table V shows that the results of the present calculation are in close agreement with the L^2 CI calculation by Moccia and Spizzo.[24] For the $2snd\ ^1D$ series, the calculated radiative lifetimes from both calculations listed in Table V are slightly longer than the model potential

TABLE III. Oscillator strengths for the $3sns\ ^1S$ to $3s3p\ ^1P$ emissions from selected theoretical calculations. The length and velocity results from Moccia and Spizzo (Ref. 17) are denoted by L and V, respectively. Both eight-state (8CC) and four-state (4CC) close-coupling results from Mendoza and Zeippen (Ref. 18) are also listed.

	ns			
Reference	4s	5s	6s	7s
Present	0.153	0.0063	0.0015	0.000 58
Froese Fischer[a]	0.155	0.0061	0.0014	0.0005
Victor, Stewart, and Laughlin[b]	0.169	0.0068	0.0019	
Moccia and Spizzo[c]—L	0.155	0.0060	0.0014	0.0005
Moccia and Spicco[c]—V	0.153	0.0058	0.0013	0.0005
Mendoza and Zeippen[d]—8CC	0.155	0.0063	0.0018	
Mendoza and Zeippen[d]—4CC	0.154	0.0063	0.0015	0.0006
Saraph[e]	0.159	0.0061	0.0014	0.0005

[a]Reference 11.
[b]Reference 12.
[c]Reference 17.
[d]Reference 18.
[e]Reference 19.

TABLE IV. Experimental and theoretical radiative lifetimes τ in ns for the excited ^3D and ^3S states of Mg I. Both length (L) and velocity (V) results from Moccia and Spizzo (Ref. 17) are listed.

Reference	τ (ns) for Mg I $3snl\ ^3L$ series				
	$3s3d\ ^3D$	$3s4d\ ^3D$	$3s5d\ ^3D$	$3s6d\ ^3D$	$3s7d\ ^3D$
Kwiatkowski, Teppner, and Zimmerman[a]	5.9±0.4	15.6±0.9	34.1±1.5	55.7±3.0	91.5±5.0
Andersen, Molhave, and Sorensen[b]	6.6±0.5	13.5±1.0			
Ueda, Karasawa, and Fukuda[c]	5.93				
Froese Fischer[d]	5.82	15.9			
Moccia and Spizzo[e]—L	5.8	15.9	33.4	59.9	98.1
Moccia and Spizzo[e]—L	5.8	15.9	33.2	59.6	95.8
Victor and Laughlin[f]	6.25	15.9			
Present	5.89	15.9	33.3	59.2	96.0
	$3s4s\ ^3S$	$3s5s\ ^3S$	$3s6s\ ^3S$	$3s7s\ ^3S$	$3s8s\ ^3S$
Schaefer[g]	14.8±0.7	25.6±2.1	52.1±6.0		
Kwiatkowski, Teppner, and Zimmerman[a]	9.7±0.6		51.8±3.0		
Andersen, Molhave, and Sorensen[b]	10.1±0.8				
Ueda, Karasawa, and Fukuda[c]	9.90±1.25				
Harvey, Balling, and Wright[h]	9.7±0.5				
Froese Fischer[d]	9.86	26.8	57.2		
Moccia and Spizzo[e]—L	9.7	26.5	56.3	104	172
Moccia and Spizzo[e]—V	9.7	26.7	56.9	104	173
Mendoza and Zeippen[i]	9.79				
Victor and Laughlin[f]	9.07				
Present	9.98	27.5	58.9	104	179

[a]Reference 4.
[b]Reference 20.
[c]Reference 21.
[d]Reference 11.
[e]Reference 17.
[f]Reference 22.
[g]Reference 3.
[h]Reference 23.
[i]Reference 18.

TABLE V. Calculated radiative lifetime τ in ns due to allowed dipole transitions for selected excited states of Be I. The length (MS-L) and velocity (MS-V) results from Moccia and Spizzo (Ref. 24) are both listed for comparison

State	Present	MS-L	MS-V	State	Present	MS-L	MS-V
$2s3s\ ^1S$	29.5	29.2	28.3	$2s3s\ ^3S$	6.65	6.70	6.52
$2s4s\ ^1S$	49.3	48.4	47.4	$2s4s\ ^3S$	17.9	18.0	17.6
$2s5s\ ^1S$	82.7	81.9	80.0	$2s5s\ ^3S$	38.4	38.4	37.2
$2s6s\ ^1S$	132	132	127	$2s6s\ ^3S$	69.9	69.6	68.5
$2s7s\ ^1S$	200			$2s7s\ ^3S$	116		
$2s2p\ ^1P$	1.73	1.79	1.86				
$2s3p\ ^1P$	54.8	63.9	70.7	$2s3p\ ^3P$	84.9	86.9	86.1
$2s4p\ ^1P$	293	289	270	$2s4p\ ^3P$	242	246	250
$2s5p\ ^1P$	308	290	273	$2s5p\ ^3P$	439	438	461
$2s6p\ ^1P$	383	361	353	$2s6p\ ^3P$	707	714	765
$2s3d\ ^1D$	12.2	12.3	12.2	$2s3d\ ^3D$	5.26	5.18	5.21
$2s4d\ ^1D$	20.1	19.9	19.8	$2s4d\ ^3D$	11.73	11.7	11.6
$2s5d\ ^1D$	35.5	35.1	34.8	$2s5d\ ^3D$	22.5		
$2s6d\ ^1D$	58.4	57.3	57.7	$2s6d\ ^3D$	38.4		
$2s7d\ ^1D$	90.1			$2s7d\ ^3D$	60.7		
$2s8d\ ^1D$	132			$2s8d\ ^3D$	90.4		

TABLE VI. Calculated transition probability A_{ij} in 10^7 sec^{-1} and branching ratio B_j in % for emissions from selected ^1P and ^1D states of Be I and Mg I.

Beryllium			Magnesium		
Transition $(i \rightarrow j)$	A_{ij}	$B_j(\%)$	Transition $(i \rightarrow j)$	A_{ij}	$B_j(\%)$
$2s4p\ ^1P \rightarrow 2s^2\ ^1S$	0.004	1.1	$3s5p\ ^1P \rightarrow 3s^2\ ^1S$	1.599	81.7
$2s4p\ ^1P \rightarrow 2s3s\ ^1S$	0.030	8.9	$3s5p\ ^1P \rightarrow 3s4s\ ^1S$	0.058	3.0
$2s4p\ ^1P \rightarrow 2s4s\ ^1S$	0.105	30.9	$3s5p\ ^1P \rightarrow 3s5s\ ^1S$	0.177	9.0
$2s4p\ ^1P \rightarrow 2p^2\ ^1D$	0.053	15.7	$3s5p\ ^1P \rightarrow 3s3d\ ^1D$	0.045	2.3
$2s4p\ ^1P \rightarrow 2s3d\ ^1D$	0.148	43.4	$3s5p\ ^1P \rightarrow 3s4d\ ^1D$	0.079	4.0
$2s3p\ ^1P \rightarrow 2s^2\ ^1S$	1.069	58.6	$3s4p\ ^1P \rightarrow 3s^2\ ^1S$	5.945	84.9
$2s3p\ ^1P \rightarrow 2s3s\ ^1S$	0.672	36.8	$3s4p\ ^1P \rightarrow 3s4s\ ^1S$	0.922	13.2
$2s3p\ ^1P \rightarrow 2p^2\ ^1D$	0.083	4.6	$3s4p\ ^1P \rightarrow 3s3d\ ^1D$	0.132	1.9
$2s2p\ ^1P \rightarrow 2s^2\ ^1S$	57.797	100.0	$3s3p\ ^1P \rightarrow 3s^2\ ^1S$	47.172	100.0
$2s5d\ ^1D \rightarrow 2s2p\ ^1P$	2.675	94.8	$3s6d\ ^1D \rightarrow 3s3p\ ^1P$	1.833	94.9
$2s5d\ ^1D \rightarrow 2s3p\ ^1P$	0.094	3.3	$3s6d\ ^1D \rightarrow 3s4p\ ^1P$	0.012	0.7
$2s5d\ ^1D \rightarrow 2s4p\ ^1P$	4×10^{-4}	~0	$3s6d\ ^1D \rightarrow 3s5p\ ^1P$	0.007	0.4
$2s5d\ ^1D \rightarrow 2s5p\ ^1P$	0.050	1.8	$3s6d\ ^1D \rightarrow 3s6p\ ^1P$	0.047	2.4
$2s5d\ ^1D \rightarrow 2s4f\ ^1F$	4×10^{-6}	~0	$3s6d\ ^1D \rightarrow 3s4f\ ^1F$	0.012	0.6
$2s5d\ ^1D \rightarrow 2s5f\ ^1F$	0.002	0.1	$3s6d\ ^1D \rightarrow 3s5f\ ^1F$	0.019	1.0
$2s4d\ ^1D \rightarrow 2s2p\ ^1P$	4.774	95.9	$3s5d\ ^1D \rightarrow 3s3p\ ^1P$	2.169	92.3
$2s4d\ ^1D \rightarrow 2s3p\ ^1P$	0.052	1.1	$3s5d\ ^1D \rightarrow 3s4p\ ^1P$	0.003	0.1
$2s4d\ ^1D \rightarrow 2s4p\ ^1P$	0.146	2.9	$3s5d\ ^1D \rightarrow 3s5p\ ^1P$	0.143	6.1
$2s4d\ ^1D \rightarrow 2s4f\ ^1F$	0.004	0.1	$3s5d\ ^1D \rightarrow 3s4f\ ^1F$	0.034	1.5
$2s3d\ ^1D \rightarrow 2s2p\ ^1P$	7.698	94.0	$3s4d\ ^1D \rightarrow 3s3p\ ^1P$	1.378	72.7
$2s3d\ ^1D \rightarrow 2s3p\ ^1P$	0.489	6.0	$3s4d\ ^1D \rightarrow 3s4p\ ^1P$	0.531	27.8
			$3s3d\ ^1D \rightarrow 3s3p\ ^1P$	1.258	100.0

TABLE VII. Calculated transition probability A_{ij} in 10^7 sec^{-1} and branching ratio B_j in % for emissions from selected ^3P and ^3D states of Be I and *Mg* I.

Beryllium			Magnesium		
Transition $(i \rightarrow j)$	A_{ij}	$B_j(\%)$	Transition $(i \rightarrow j)$	A_{ij}	$B_j(\%)$
$2s5p\ ^3P \rightarrow 2s3s\ ^3S$	1.5×10^{-4}	0.1	$3s6p\ ^3P \rightarrow 3s4s\ ^3S$	0.038	22.6
$2s5p\ ^3P \rightarrow 2s4s\ ^3S$	0.010	4.2	$3s6p\ ^3P \rightarrow 3s5s\ ^3S$	0.037	21.5
$2s5p\ ^3P \rightarrow 2s5s\ ^3S$	0.051	22.4	$3s6p\ ^3P \rightarrow 3s6s\ ^3S$	0.063	37.2
$2s5p\ ^3P \rightarrow 2s3d\ ^3D$	0.081	35.8	$3s6p\ ^3P \rightarrow 3s3d\ ^3D$	0.016	9.4
$2s5p\ ^3P \rightarrow 2s4d\ ^3D$	0.086	37.5	$3s6p\ ^3P \rightarrow 3s4d\ ^3D$	0.016	9.3
			$3s6p\ ^3P \rightarrow 3s5d\ ^3D$	3.7×10^{-6}	~0
$2s4p\ ^3P \rightarrow 2s3s\ ^3S$	0.016	3.8	$3s5p\ ^3P \rightarrow 3s4s\ ^3S$	0.130	32.9
$2s4p\ ^3P \rightarrow 2s4s\ ^3S$	0.192	46.4	$3s5p\ ^3P \rightarrow 3s5s\ ^3S$	0.224	57.4
$2s4p\ ^3P \rightarrow 2s3d\ ^3D$	0.206	49.8	$3s5p\ ^3P \rightarrow 3s3d\ ^3D$	0.038	9.7
			$3s5p\ ^3P \rightarrow 3s4d\ ^3D$	1.3×10^{-5}	~0
$2s3p\ ^3P \rightarrow 2s3s\ ^3S$	1.178	100.0	$3s4p\ ^3P \rightarrow 3s4s\ ^3S$	12.970	100.0
$2s5d\ ^3D \rightarrow 2s2p\ ^3P$	4.068	91.4	$3s5d\ ^3D \rightarrow 3s3p\ ^3P$	2.325	77.5
$2s5d\ ^3D \rightarrow 2s3p\ ^3P$	0.310	7.0	$3s5d\ ^3D \rightarrow 3s4p\ ^3P$	0.455	15.2
$2s5d\ ^3D \rightarrow 2s4p\ ^3P$	0.047	1.1	$3s5d\ ^3D \rightarrow 3s5p\ ^3P$	0.204	6.8
$2s5d\ ^3D \rightarrow 2s5p\ ^3P$	0.013	0.3	$3s5d\ ^3D \rightarrow 3s4f\ ^3F$	0.016	0.5
$2s5d\ ^3D \rightarrow 2s4f\ ^3F$	0.011	0.2			
$2s4d\ ^3D \rightarrow 2s2p\ ^3P$	8.055	94.5	$3s4d\ ^3D \rightarrow 3s3p\ ^3P$	5.282	84.0
$2s4d\ ^3D \rightarrow 2s3p\ ^3P$	0.428	5.0	$3s4d\ ^3D \rightarrow 3s4p\ ^3P$	1.005	16.0
$2s3d\ ^3D \rightarrow 2s2p\ ^3P$	18.816	99.0	$3s3d\ ^3D \rightarrow 3s3p\ ^3P$	16.972	100.0
$2s3d\ ^3D \rightarrow 2s2p\ ^3P$	0.198	1.0	$3s3d\ ^3D \rightarrow 3s4p\ ^3P$	1×10^{-5}	~0

TABLE VIII. Radiative lifetimes τ in ns for the excited $^{1,3}P$ states of Mg I from selected theoretical calculations.

State	Present	Froese Fischer[a]	Moccia and Spizzo[b]	
			Length	Velocity
$3s3p\ ^1P$	2.12	2.08	2.17	2.15
$3s4p\ ^1P$	14.3	14.0	14.3	14.3
$3s5p\ ^1P$	51.5	48.9	49.3	50.6
$3s6p\ ^1P$	121	116	118	119
$3s7p\ ^1P$	235	216	228	227
$3s4p\ ^3P$	77	80	81	81
$3s5p\ ^3P$	256	269	276	278
$3s6p\ ^3P$	5.9×10^2	6.2×10^2	6.5×10^2	6.5×10^2
$3s7p\ ^3P$	1.1×10^3		1.2×10^3	1.2×10^2

[a]Reference 11.
[b]Reference 17.

results listed in Table 4 of Ref. 22. A detailed comparison of the previous theoretical and experimental lifetimes is given recently by Moccia and Spizzo.[24] Similar to the Mg I $3sns\ ^{1,3}S$ series, the accuracy of the calculated lifetimes of the higher excited Be I $2sns\ ^{1,3}S$ states also suffers from the combination of large branching ratios and small oscillator strengths for the $2sns\ ^{1,3}S\rightarrow 2s2p\ ^{1,3}P$ emissions. The transition probabilities and the corresponding branching ratios for emissions from selected Be I $2nsn\ ^{1,3}S$ states are listed in Table II. The lifetimes of the higher $2snp\ ^3P$ states are calculated without the *near zero* contributions from the $2snp\ ^3P^0\rightarrow 2p^2\ ^3P^e$ emissions.[24] For the Be I $2snd\ ^{1,3}D$ series, the radiative decay is dominated by the $2snd\ ^{1,3}D\rightarrow 2s2p\ ^{1,3}P$ emissions as shown by the transition probabilities listed in Tables VI and VII. For the first few low-lying $2snd\ ^{1,3}D$ states, the oscillator strengths are relatively large.[15] As a result, the calculated radiative lifetimes are more reliable for the first few $^{1,3}D$ states.

In Tables VI and VII, we also list the transition probabilities and the branching ratios for selected Be I $2snp\ ^{1,3}P$ and Mg I $3snp\ ^{1,3}P$ states. Similar to the ^1S states shown in Table II, the radiative decay from the Be I $2snp\ ^{1,3}P$ and the Mg I $3snp\ ^3P$ states cannot be identified with a single dominating emission. In contrast, the radiative decay from an excited Mg I $3snp\ ^1P$ state is dominated by the $3snp\ ^1P\rightarrow 3s^2\ ^1S$ emission in spite of its small oscillator strength.[15] The presence of the $2p^2\ ^1D$ state and the relatively large mixing between $2s^2$ and $2pp\ ^1S$ configuration series are responsible for the somewhat different radiative decay pattern for the higher ^1P states between Be I and Mg I as shown by the branching ratios listed in Table VI. Our calculation has also shown that for the higher Be I $2snp\ ^3P$ states, the $^3P\rightarrow{}^3D$ emissions are the more probable decay mode than the $^3P\rightarrow{}^3S$ emissions whereas for the Mg I $3snp\ ^3P$ states, the $^3P\rightarrow{}^3S$ emissions are the more favorable decay mode as shown by the branching ratios listed in Table VII. Finally, Table VIII shows that the agreement between theoretical radiative lifetimes of Mg I $^{1,3}P$ states are generally very good. Again, we note that the *near zero* contributions to the radiative lifetimes of the higher $3snp\ ^3P$ states from the $3snp\ ^3P^0\rightarrow 3p^2\ ^3P^e$ emissions are not included in the theoretical calculations. A more detailed comparison between theoretical and experimental lifetimes of the Mg I $^{1,3}P$ states are given recently by Moccia and Spizzo in Ref. 17.

In summary, the present study has demonstrated that the simple CI procedure, with configurations represented by two-electron L^2 basis sets constructed from B splines, is capable of leading to theoretical radiative lifetimes which are in good agreement with the most accurate state-selected excitation measurements. Extension of this simple CI procedure to the transition probabilities and the radiative lifetimes of the Be and Mg isoelectronic sequence is currently in progress.

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