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Large-scale relativistic configuration-interaction calculation of the $3s^{2\,1}S_0$-$3s3p\ ^{1,3}P_1$ transition energies in magnesiumlike ions

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We have calculated the $3s^{2\,1}S_0$-$3s3p\ ^{1,3}P_1$ transition energies for neutral magnesium and Mg-like Ar^{6+}, Cu^{17+}, Kr^{24+}, and Mo^{30+} using the relativistic configuration-interaction (CI) method. These calculations are based on the relativistic no-pair Hamiltonian which includes Coulomb and retarded Breit interactions and employ finite B-spline basis functions. Quantum electrodynamic and mass polarization corrections are also calculated. For Mg-like ions studied here, intravalence correlations are treated exactly by saturating the basis with all configurations that arise from valence-valence excitations. Contributions from core polarization are also calculated with large-scale CI expansions by including dominant configurations from core-valence excitations. Agreement between theory and experiment are good for all the Mg-like ions studied here. [S1050-2947(97)02305-6]

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I. INTRODUCTION

Advances in experimental techniques in producing highly charged heavy ions have led to many precision experiments on energy levels of high-Z ions [1–5]. These highly accurate experimental results have stimulated the development of theory to tackle the relativistic correlation problem [6–14] and to improve the treatment of quantum electrodynamic (QED) corrections for many-electron ions [15–17]. Recently, several accurate systematic calculations of energy levels for He-like to Na-like ions have been carried out using the relativistic many-body perturbation theory (MBPT) [6–9], and the relativistic configuration-interaction (CI) method with B-spline basis sets [10–14]. So far, these studies are limited either to few-electron ions or to alkalilike systems.

Energies and oscillator strengths for the $n=3$-3 transitions in Mg-like ions have been subjected to many theoretical and experimental investigations. Numerous experimental data for the M-shell transitions in the Mg sequence can be found in the literature [18–25]. On the theoretical front, many calculations have been carried out for the transition energies between M-shell levels using, for example, the Hartree-Fock (HF) method [26,27], the multiconfiguration Dirac-Fock (MCDF) method [19,28,29], and the multiconfiguration relativistic random-phase approximation (MCRRPA) [30,31]. Most of these existing calculations included only valence-valence correlations and QED corrections are either completely ignored or taken into account phenomenologically. The effects of core-valence correlations have been considered before, but largely through the use of semiempirical, core-polarization model potentials in nonrelativistic CI calculations [32–36].

Two recent relativistic calculations include more rigorous treatments of core-valence correlations: the MCRRPA method of Chou, Chi, and Huang [31], which includes electric-dipole excitation channels from the $n=2$ shell to account for core-polarization effects, and the MCDF+CP method of Stanek, Glowacki, and Migdalek [29], which employs model potentials with *ab initio* core-polarization parameters in MCDF calculations. For low-Z Mg-like ions, Stanek, Glowacki, and Migdalek [29] also use a CIDF+CP method which is similar to MCDF+CP but is based on CI calculations with Dirac-Fock basis functions. The MCRRPA method is known to give reliable, gauge invariant oscillator strengths but is not as suitable for high-precision transition energy calculations, as it does not include all correlation terms that arise from perturbation theory. As for the MCDF+CP and CIDF+CP methods, even though no semiempirical parameters are used, they still rely on model potentials to account for core-polarization effects and thus remain approximated treatments only. To date, residual discrepancies between theory and experiment on the $3s^{2\,1}S_0$-$3s3p\ ^{1,3}P_1$ excitation energies remain high and are as much as a few thousand wave numbers for low- to mid-Z Mg-like ions.

In this work, we apply the relativistic CI method to calculate the $3s^{2\,1}S_0$-$3s3p\ ^{1,3}P_1$ transition energies for Mg, Ar, Cu, Kr, and Mo ions in the magnesium isoelectronic sequence. Our calculations are based on the relativistic no-pair Hamiltonian and use finite, B-spline orbitals as basis functions. All configurations that arise from single and double excitations of the two valence electrons are included. In addition, contributions from core polarizations are calculated with large-scale CI expansions using dominant configurations from core-valence excitations. To our knowledge, this is the most extensive calculation of core-valence corrections in Mg-like ions to date. For accurate transition energy results, *ab initio* QED and mass polarization corrections are also included. Resulting agreement between theory and experiment is good, and is consistently better than 100 cm^{-1} for all the Mg-like ions studied here.

II. THEORETICAL CALCULATION

In the present work, we employ the relativistic no-pair Hamiltonian for an N-electron system which is given by [37,38]

$$H=\sum_{i=1}^{N} h_0(i)+\Lambda_{++}(H_C+H_B)\Lambda_{++}. \quad (1)$$

Here, h_0 is the single-particle Dirac Hamiltonian for an electron moving in a nuclear Coulomb potential represented by a two-parameter Fermi charge distribution of the nucleus, Λ_{++} is the positive-energy projection operator, and H_C and H_B are the Coulomb and retarded Breit interactions, respectively. The eigenfunction $\Psi(JM)$ of an atomic state with angular momentum (J,M) and parity π is expressed as a linear combination of the many-electron configuration-state functions $\phi(\Gamma_K JM)$

$$\Psi(JM)=\sum_K c_K \phi(\Gamma_K JM), \quad (2)$$

where Γ_K is a set of quantum numbers representing different electronic configurations, and c_K is the mixing coefficient. Variation of the energy functional $\langle\Psi|H|\Psi\rangle$ with respect to c_K, subjected to the wave function normalization condition, leads to the CI equation

$$\sum_L (H_{KL}-\lambda\,\delta_{KL})c_L=0. \quad (3)$$

Details of the theory and expressions for the Coulomb and Breit matrix elements for H_{KL} in terms of the configuration-state functions $\phi(\Gamma JM)$ can be found in Refs. [10–12].

In this work, many-electron, configuration-state functions are constructed from one-electron, B-spline basis functions which are solutions of the Dirac equation for an electron moving in a model potential confined to a finite cavity. These B-spline functions are obtained using the method by Johnson, Blundell, and Sapirstein [39]. Model potentials used here are Dirac-Slater (DS) potentials with Kohn-Sham exchanges for the $3s^2$ ground state of Mg-like ions. Parameters for the Fermi charge distribution of the nucleus are taken from Johnson and Soff [40]. A cavity radius of 50 a.u. is used for neutral magnesium. This radius is gradually reduced with increasing Z, from 6 a.u. for Ar^{6+} to 2.5 a.u. for Mo^{30+}. Also, 30 positive-energy and 30 negative-energy B-spline orbitals are generated for each of the $s, p, d, \ldots$ states inside the cavity. Only positive-energy B-spline orbitals are used here, in compliance with the positive-energy projection operators in the no-pair Hamiltonian. In particular, only the first 19 out of 30 positive-energy orbitals for each of the angular symmetries are used, as contributions from the remaining orbitals are quite negligible. We include orbitals with $\ell=0-5$. Contributions from higher partial waves are taken into account by extrapolations.

In our CI expansions, configuration-state functions (CSFs) include states that arise from single and double excitations from the reference states $1s^2 2s^2 2p^6 3s^2 + 1s^2 2s^2 2p^6 3p^2 (J=0)$ and $1s^2 2s^2 2p^6 3s3p (J=1)$. The basic sets of CSFs include all configurations that arise from the valence-valence excitations

$$1s^2 2s^2 2p^6 n\ell n'\ell'.$$

To account for core-polarization effects, additional CSFs are included. In this case, single excitations are from the $1s^2 2s^2 2p^6$ Ne-like core only, while double excitations are restricted to core-valence excitations, with one electron from the Ne-like core while the other is from the valence shells. Contributions from core-core excitations, which are common to the initial and final states, should be largely canceled in transition energy calculations and are neglected here. Depending on which of the core electron is getting excited, CSFs for core-valence excitations thus consist of the following groups of configurations:

$$\begin{aligned} 2p \text{ excitations:}\quad & 1s^2 2s^2 2p^5 3sn\ell n'\ell', \\ & 1s^2 2s^2 2p^5 3pn\ell n'\ell', \\ 2s \text{ excitations:}\quad & 1s^2 2s\, 2p^6 3sn\ell n'\ell', \\ & 1s^2 2s\, 2p^6 3pn\ell n'\ell', \\ 1s \text{ excitations:}\quad & 1s\, 2s^2 2p^6 3sn\ell n'\ell', \\ & 1s\, 2s^2 2p^6 3pn\ell n'\ell'. \end{aligned}$$

As the same CSFs can arise from different groups of excitations (e.g., $3s3p3d$ from $3sn\ell n'\ell'$ is the same as $3p3s3d$ from $3pn\ell n'\ell'$), care is taken to ensure that there are no ‘‘double countings’’ of CSFs throughout this work.

To carry out CI calculations with $\ell=0-5$, the basic, valence-valence excitation calculations consist of a few thousand CSFs and pose no particular problem. When core electrons are allowed to get excited, however, the number of CSFs can become prohibitively large. To make the problem numerically tractable, core-valence correlation calculations are broken down into more manageable pieces. Specifically, each group of CSFs from the core-valence excitations, shown above, is paired with the basic set of CSFs from the valence-valence excitations. The contribution to the correlation energy from this group of core-valence excitations is then obtained by taking the difference between the paired calculation and the basic, valence-valence excitation calculation. To further control the size of these calculations, contributions from CSFs with $\Delta\ell=|\ell-\ell'|\leqslant 1$ ($nsns$, $nsnp$, $\ldots$) and those with $\Delta\ell=2$ ($nsnd$, $npnf$, $\ldots$) are calculated separately. Contributions from $\Delta\ell\geqslant 3$ are very small and are not considered here.

In this work, we also include contributions from the most important triple excitations from the reference states. These triply excited CSFs come from the excitations of a single core electron along with both of the valence electrons and are given by

$$1s^2 2s^2 2p^5 3dn\ell n'\ell', \quad 1s^2 2s^2 2p^5 4sn\ell n'\ell',$$

$$1s^2 2s\, 2p^6 4sn\ell n'\ell', \quad 1s\, 2s^2 2p^6 4sn\ell n'\ell',$$

with $n,n'\geqslant 4$. For the $3s3p\ {}^{1,3}P_1$ states, the following group of triply excited CSFs is also included

$$1s^2 2s^2 2p^5 4pn\ell n'\ell'.$$

The contribution from each group of triple excitations is calculated separately using the same procedure mentioned earlier for the evaluation of core-valence excitations. As contributions from triple excitations are small, we limit these

TABLE I. Coulomb and Breit energies (a.u.) of the $3s^2\,{}^1S_0$-$3s3p\,{}^{1,3}P_1$ transitions in Mg-like ions. The third column shows transition energies including valence-valence correlations only. The fourth to sixth columns are contributions from core-valence interactions with the excitation of a $2p$, $2s$, and $1s$ core electron, respectively. The seventh column represents contributions from triple excitations.

Interaction	Z	Valence	$2p$	$2s$	$1s$	Triple	Sum
				$3s^2\,{}^1S_0$-$3s3p\,{}^3P_1$			
Coulomb	12	0.096 90	0.003 93	0.000 53	0.000 06	−0.001 81	0.099 61
	18	0.515 30	0.004 62	−0.001 16	0.000 10	−0.000 00	0.518 86
	29	1.316 64	0.005 10	−0.001 71	−0.000 21	−0.000 00	1.319 82
	36	1.878 55	0.004 71	−0.001 77	−0.000 16	−0.000 00	1.881 33
	42	2.394 61	0.004 09	−0.001 82	−0.000 12	−0.000 00	2.396 76
Breit	12	−0.000 02					−0.000 02
	18	0.000 21	0.000 03	0.000 03	0.000 02		0.000 29
	29	0.003 21	−0.000 18	0.000 08	0.000 04		0.003 15
	36	0.008 57	−0.000 32	0.000 09	0.000 06		0.008 40
	42	0.016 51	−0.000 48	0.000 07	0.000 05		0.016 15
				$3s^2\,{}^1S_0$-$3s3p\,{}^1P_1$			
Coulomb	12	0.158 70	0.001 51	0.000 45	0.000 24	−0.001 28	0.159 62
	18	0.785 19	−0.005 87	−0.001 23	0.000 19	−0.000 02	0.778 26
	29	1.961 67	−0.010 25	−0.001 95	−0.000 18	−0.000 01	1.949 28
	36	2.903 06	−0.010 70	−0.002 04	−0.000 12	−0.000 00	2.890 20
	42	3.958 48	−0.010 18	−0.002 08	0.000 01	−0.000 00	3.946 23
Breit	12	−0.000 04					−0.000 04
	18	−0.000 03	0.000 02	0.000 02	0.000 02		0.000 03
	29	0.000 91	−0.000 23	0.000 01	0.000 08		0.000 77
	36	0.001 84	−0.000 43	−0.000 01	0.000 06		0.001 46
	42	0.002 44	−0.000 66	−0.000 04	0.000 01		0.001 75

calculations to $\ell,\ell' \leqslant 2$ only. Also, these calculations are carried out for the Coulomb interaction only, as contributions from the Breit interaction are quite negligible.

As in previous relativistic CI calculations for Be-like ions [14], off-diagonal Hamiltonian matrix elements from single and double excitations are evaluated with the unretarded Breit operator, while diagonal matrix elements are calculated with the retarded Breit operator to obtain the leading frequency-dependent corrections to the Breit energies. Since contributions from the retarded Breit interaction to the $3s^2\,{}^1S_0$-$3s3p\,{}^{1,3}P_1$ transition energies come mainly from the $1s^2$ core and are largely canceled between the initial and final states, the effect of neglecting retardation in the off-diagonal Breit matrix elements is expected to be rather insignificant.

The dimensions of the real, symmetric matrices encountered in our present CI calculations range from 2000 to 30 000 even after breaking up the problem into smaller pieces. In double-precision, symmetric storage mode, these matrices can take up to 4 gigabytes of on-line hard disk space. An iterative Davidson's method [41] as implemented by Stathopoulos and Froese Fischer [42] is used to solve for the first few eigenvalues of the CI equation. This method is very efficient for diagonally dominated matrices like the ones we have here. In general, no more than ten iterations are needed to achieve convergence. These are large-scale, computer-intensive calculations. Even with heavy optimization of the computer codes, a typical job here can take over 15 hours of CPU time and run for days on supercomputers like the Cray-YMP.

In the present work, mass polarization corrections are calculated as first-order perturbations with the operator $H_{\mathrm{MP}}=1/M\Sigma_{i<j}\mathbf{p}_i\cdot\mathbf{p}_j$, where M is the nuclear mass, using eigenvectors from our CI calculations. Also, one-electron self-energies for the $3s$ and $3p$ orbitals are calculated using the scheme of Cheng, Johnson, and Sapirstein [15]. The effects of electron screening and nuclear finite size are included by using the same DS potential as in the CI calculations. Leading vacuum polarization corrections are evaluated as expectation values of the Uehling potential. Total QED correction for a many-electron eigenstate is then given by the sum of the single-particle QED corrections, weighted by the fractional occupation number of each orbital as obtained from the eigenvector of the CI calculation.

III. RESULTS AND DISCUSSION

In Table I, contributions from valence-valence, core-valence, and triple excitations to the Coulomb and Breit energies of the $3s^2\,{}^1S_0$-$3s3p\,{}^{1,3}P_1$ transitions are shown for Mg, Ar^{6+}, Cu^{17+}, Kr^{24+}, and Mo^{30+}. Results from $\Delta\ell \leqslant 1$ and $\Delta\ell=2$ are combined here. In general, contributions from CSFs with $\Delta\ell=2$ are much smaller than those with $\Delta\ell\leqslant 1$. The only exception is the group of CSFs from $1s^2 2s^2 2p^5 3sn\ell n'\ell'$ with $\Delta\ell=2$, which contributes heavily to the correlation energies of the $3s3p\,{}^{1,3}P_1$ states. In particular, term energies are lowered by $-0.002\,84$ a.u. for the ${}^3P_1$ state and by $-0.009\,25$ a.u. for the ${}^1P_1$ state in Ar^{6+}. Corresponding values for Mo^{30+} are $-0.005\,31$ and $-0.013\,72$ a.u., respectively.

From Table I, it can be seen that valence-valence excitations account for over 99% of the transition energies for

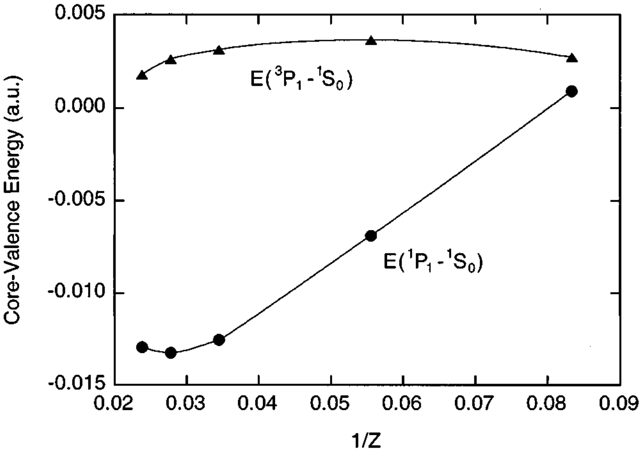

FIG. 1. Core-valence energies (a.u.) of the $3s^2\,{}^1S_0$-$3s3p\,{}^{1,3}P_1$ transitions from the present CI calculations are plotted as functions of 1/Z.

most of these Mg-like ions. However, for high-precision calculations, contributions from core-valence excitations cannot be ignored, especially at low Z. As expected, core-valence contributions come mainly from the $2p$ shell, which is more easily polarized, followed by the $2s$ shell and the $1s$ shell. While excitation energies scale like Z for these $\Delta n=0$ transitions, core-valence energies remain fairly constant along the isoelectronic sequence and become less important for high-Z ions. This is consistent with the relativisitic 1/Z expansion analysis: With all configurations in the $n=3$ complex included, our valence-valence results are exact to terms that are linear in Z in 1/Z series expansions. As a result, core-valence contributions should behave like

$$a_{00}+a_{01}/Z+\cdots+a_{10}(\alpha Z)^2+\cdots.$$

As shown in Fig. 1, where the core-valence energies of the $3s^2\,{}^1S_0$-$3s3p\,{}^{1,3}P_1$ transitions are plotted as functions of 1/Z, our results are indeed consistent with this prediction. In particular, core-valence energies for the ${}^1P_1$ transition clearly show a 1/Z behavior at low Z, until the leading relativistic corrections from the $(\alpha Z)^2$ term take over at higher Z. Core-valence energies for the ${}^3P_1$ transition are seen to be smaller in size and vary more slowly along the isoelectronic sequence.

One can also see that contributions to the correlation energy from configurations arising from triple excitations are important only for low-Z ions. In fact, triple excitations affect the excited states more than the ground state. For neutral magnesium, for example, the ground state is lowered by $-0.000\,07$ a.u. while the ${}^3P_1$ and ${}^1P_1$ excited states are changed by $-0.001\,88$ and $-0.001\,35$ a.u., respectively. Contributions from other uncalculated triple and quadruple excitations are expected to be less than 1×10^{-4} a.u.

It should be pointed out that what classified as triple excitations depends, to some extent, on what we define as the reference states. For the $3s^2\,{}^1S_0$ ground state, by including the $1s^2 2s^2 2p^6 3p^2(J=0)$ configuration in the reference state, $1s^2 2s^2 2p^5 3pn\ell n'\ell'$, $1s^2 2s 2p^6 3pn\ell n'\ell'$, and $1s 2s^2 2p^6 3pn\ell n'\ell'$ configurations are classified as double excitations instead of triple excitations. This is necessary because contributions from these CSFs to the correlation energy of the ground state are substantial, and amount to $-0.001\,09$, $-0.001\,75$, and $-0.001\,02$ a.u. for Mg, Ar^{6+}, and Mo^{30+}, respectively. On the other hand, the $1s^2 2s^2 2p^6 3d^2(J=0)$ configuration, though known to be important for intravalence correlations and is included in our valence-valence calculations, is not considered as part of the reference state. This is because core-valence excitations from this state do not contribute much to the correlation energies. As a result, these excitations (e.g., $1s^2 2s^2 2p^5 3dn\ell n'\ell'$) are classified as triple excitations here.

There are several issues concerning the numerical calculations that need to be addressed. As mentioned earlier, we use only 19 out of 30 B-spline functions for each angular symmetry in the calculation. In fact, eigenenergies are found to converge to 1×10^{-6} a.u. after including the first 17 orbitals in CI expansions. The extra two orbitals are added to ensure this level of convergence throughout our calculations. Furthermore, the accuracy of the B-spline basis functions is checked by varying the cavity size up to a factor of 2, as well as by generating 40 B-spline orbitals for each angular symmetry instead of the usual 30 and using the first 25 in CI calculations. All these tests indicate that our CI energies are stabilized to better than 1×10^{-5} a.u.

Another point to be made is that while results of a full CI calculation should be independent of the model potential used to generate B-spline basis functions, individual contributions to the correlation energy from valence-valence, core-valence, triple, etc. excitations are, nevertheless, potential dependent. This was demonstrated in previous CI calculations for Be-like ions [14], where results from different model potentials were compared. In Ref. [14], it was found that four-electron DS potentials consistently minimize contributions from small corrections like triple excitations, thus reducing computational efforts and ensuring better numerical accuracies. We expect the same to be true here. While we do not completely saturate the basis with all configurations from multiple excitations in a Mg-like ion, numerical uncertainties from using 12-electron DS potentials in our present calculations are expected to be small, at less than 1×10^{-4} a.u.

Perhaps the biggest errors in our calculations come from the treatment of core polarizations. To begin with, core-core excitations are ignored here and their contributions to the transition energy can amount to 1×10^{-4} a.u. More importantly, by calculating core-valence contributions from different groups of CSFs separately as explained in the preceding section, interactions between groups of core-valence excitations are ignored. While these are small, higher-order corrections, tests show that they can give rise to theoretical uncertainties of the order of a few times 10^{-4} a.u. Overall, we expect our CI results to be accurate to this level, which is about 100 cm^{-1}.

In Table II, we list Coulomb, Breit, QED, and mass polarization (MP) contributions to the energies of the $3s^2\,{}^1S_0$-$3s3p\,{}^{1,3}P_1$ transitions for Mg, Ar^{6+}, Cu^{17+}, Kr^{24+}, and Mo^{30+}. Coulomb and Breit energies listed here include all contributions from valence-valence, core-valence, and triple excitations as shown in Table I. While our QED results included lowest-order radiative corrections only, uncertainties arising from the use of DS potentials to account for screen-

TABLE II. Coulomb, Breit, QED, and mass polarization (MP) contributions to the total CI energies (a.u.) of the $3s^2\,{}^1S_0$-$3s3p\,{}^{1,3}P_1$ transitions in Mg-like ions.

Z	Coulomb	Breit	QED	MP	Total
$3s^2\,{}^1S_0$-$3s3p\,{}^3P_1$					
12	0.099 61	−0.000 02	−0.000 10	−0.000 00	0.099 49
18	0.518 86	0.000 29	−0.000 53	−0.000 02	0.518 60
29	1.319 82	0.003 15	−0.004 66	−0.000 09	1.318 22
36	1.881 33	0.008 40	−0.011 26	−0.000 12	1.878 35
42	2.396 76	0.016 15	−0.020 64	−0.000 15	2.392 12
$3s^2\,{}^1S_0$-$3s3p\,{}^1P_1$					
12	0.159 62	−0.000 04	−0.000 10	−0.000 00	0.159 48
18	0.778 26	0.000 03	−0.000 53	−0.000 02	0.777 74
29	1.949 28	0.000 77	−0.004 57	−0.000 08	1.945 40
36	2.890 20	0.001 46	−0.010 78	−0.000 12	2.880 76
42	3.946 23	0.001 75	−0.019 40	−0.000 14	3.928 44

ing corrections are expected to be small compared to those from the CI calculations for the Mg-like ions studied here.

In Table III, energies of the ${}^{1,3}P_1$ states relative to the ground state from the present work are compared with other relativistic calculations [19,29,31] and with experiment [18–20]. There are two CI values here: CI(VV) includes valence-valence correlations only while full CI includes core-valence correlations in addition. Both of them have the same QED and MP corrections as shown in Table II. Also shown are results from three existing relativistic calculations: MCRRPA of Chou, Chi, and Huang [31], MCDF+CP–CIDF+CP of Stanek, Glowacki, and Migdalek [29], which include some contributions from core polarizations as mentioned in Sec. I, and MCDF of Sugar *et al.* [19], which includes valence-valence excitations only. Our CI(VV) results are comparable in accuracy to other existing theories and differ from experiment by as much as 900 cm^{-1} for the ${}^3P_1$ and 3000 cm^{-1} for the ${}^1P_1$ states. Including core-valence correlations in our present CI calculations improves the agreement with experiment to better than 100 cm^{-1} for both transitions in all ions covered in this study.

More detailed comparisons between theory and experiment on the transition energies of $3s^2\,{}^1S_0$-$3s3p\,{}^{1,3}P_1$ are shown in Figs. 2 and 3. In spite of the fact that MCRRPA [31] and MCDF+CP–CIDF+CP [29] include some contributions from core-valence correlations, it can be seen that, in general, these results are not any better than our CI(VV) results which include valence-valence correlations only. From these two figures, it can also be seen that differences between existing theories [19,29,31] and experiment remain large and range from 300 cm^{-1} to 4000 cm^{-1}, while our full CI results consistently agree very well with experiment

TABLE III. Energies of the $3s3p\,{}^{1,3}P_1$ states relative to the ground state in cm^{-1}. Here, CI(VV) are the present results with valence-valence correlations only while full CI are results that include core-valence correlations also. Other calculations listed here are MCRRPA by Chou, Chi, and Huang [31], MCDF+CP and CIDF+CP by Stanek, Glowacki, and Migdalek [29] and MCDF by Sugar *et al.* [19].

Z	CI(VV)	Full CI	MCRRPA	Ref. [29]	MCDF	Experiment	Reference
$3s^2\,{}^1S_0$-$3s3p\,{}^3P_1$							
12	21 260	21 835	20 901	21 322 [a]		21 870	[18]
18	112 996	113 818	113 326	112 746 [b]		113 899	[18]
29	288 591	289 313			288 550	289 401(4)	[19]
36	411 636	412 247				412 290(8)	[19]
						412 233 (55)	[20]
42	524 573	525 007			524 721	525 028 (14)	[19]
						525 024 (48)	[20]
$3s^2\,{}^1S_0$-$3s3p\,{}^1P_1$							
12	34 832	35 001		35 230 [a]		35 051	[18]
18	172 240	170 692	171 704	173 896 [b]		170 718	[18]
29	429 771	426 962			430 956	426 987(9)	[19]
36	635 216	632 250				632 187 (20)	[19]
						632 178 (47)	[20]
42	865 089	862 188			866 229	862 076 (37)	[19]
						862 110 (94)	[20]

[a] CIDF+CP results.

[b] MCDF+CP results.

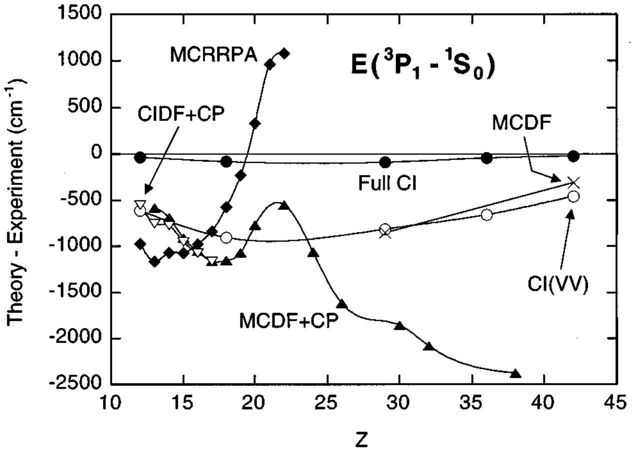

FIG. 2. The $3s^2\,{}^1S_0$-$3s3p\,{}^3P_1$ transition energies (cm^{-1}) relative to experiment are shown as functions of Z. Open and closed circles are CI(VV) and full CI results of this work. Diamonds, triangles, inverted triangles, and crosses are MCRRPA [31], MCDF+CP [29], CIDF+CP [29], and MCDF [19] results, respectively. Experimental errors are smaller than the size of the symbols and are not shown here.

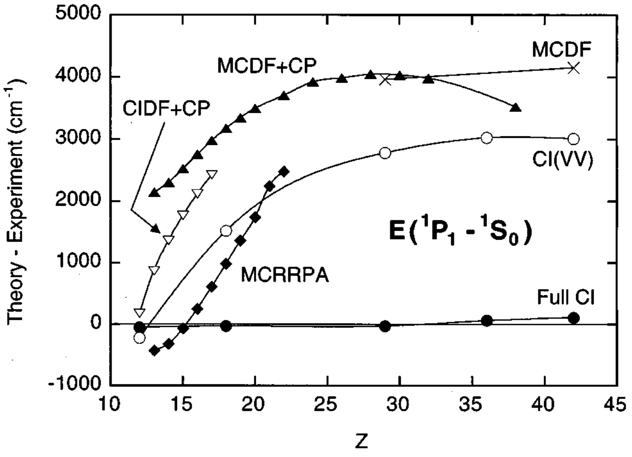

FIG. 3. The $3s^2\,{}^1S_0$-$3s3p\,{}^1P_1$ transition energies (cm^{-1}) relative to experiment are shown as functions of Z. Symbols are the same as those in Fig. 2.

for all Mg-like ions considered here.

In summary, we have carried out relativistic CI calculations using B-spline basis functions for the correlation energies of the $3s^2\,{}^1S_0$-$3s3p\,{}^{1,3}P_1$ transitions in neutral magnesium and Mg-like Ar^{6+}, Cu^{17+}, Kr^{24+}, and Mo^{30+}. We have found that core-valence correlations are essential in removing residual discrepancies between theory and experiment. In addition, we have shown that the procedure of breaking the problem into smaller, more manageable calculations does work and can yield highly accurate transition energy results. This demonstrates the feasibility of carrying out large-scale CI calculations for many-electron systems.

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[1] J. F. Seely, U. Feldman, C. M. Brown, M. C. Richardson, D. D. Dietrich, and W. E. Behring, J. Opt. Soc. Am. B **5**, 785 (1988).

[2] D. D. Dietrich, A. Simionovici, M. H. Chen, G. Chandler, C. J. Hailey, P. O. Egan, P. H. Mokler, S. Reusch, and D. H. H. Hoffmann, Phys. Rev. A **41**, 1450 (1990).

[3] J. F. Seely, C. M. Brown, U. Feldman, J. O. Ekberg, C. J. Keane, B. J. MacGowan, D. R. Kania, and W. E. Behring, At. Data Nucl. Data Tables **47**, 1 (1991).

[4] P. Beiersdorfer, D. Knapp, R. E. Marrs, S. R. Elliott, and M. H. Chen, Phys. Rev. Lett. **71**, 3939 (1993).

[5] P. Beiersdorfer, A. Osterheld, S. R. Elliott, M. H. Chen, D. Knapp, and K. Reed, Phys. Rev. A **52**, 2693 (1995).

[6] W. R. Johnson, S. A. Blundell, and J. Sapirstein, Phys. Rev. A **37**, 2764 (1988); **38**, 2699 (1988); **42**, 1087 (1990).

[7] W. R. Johnson and J. Sapirstein, Phys. Rev. A **46**, R2197 (1992).

[8] D. R. Plante, W. R. Johnson, and J. Sapirstein, Phys. Rev. A **49**, 3519 (1994).

[9] W. R. Johnson, J. Sapirstein, and K. T. Cheng, Phys. Rev. A. **51**, 297 (1995).

[10] M. H. Chen, K. T. Cheng, and W. R. Johnson, Phys. Rev. A **47**, 3692 (1993).

[11] K. T. Cheng, M. H. Chen, W. R. Johnson, and J. Sapirstein, Phys. Rev. A **50**, 247 (1994).

[12] M. H. Chen, K. T. Cheng, W. R. Johnson, and J. Sapirstein, Phys. Rev. A **52**, 266 (1995).

[13] K. T. Cheng and M. H. Chen, Phys. Rev. A **53**, 2206 (1996).

[14] M. H. Chen and K. T. Cheng, Phys. Rev. A. **55**, 166 (1997).

[15] K. T. Cheng, W. R. Johnson, and J. Sapirstein, Phys. Rev. A **47**, 1817 (1993); Phys. Rev. Lett. **66**, 2960 (1991).

[16] S. A. Blundell and N. Snyderman, Phys. Rev. A **44**, R1427 (1991); S. A. Blundell, Phys. Rev. A **47**, 1790 (1993).

[17] I. Lindgren, H. Persson, S. Salomonson, and A. Ynnerman, Phys. Rev. A **47**, R4555 (1993).

[18] C. E. Moore, *Atomic Energy Levels*, Natl. Bur. Stand. (U.S.) Circ. No. NSRDS-NBS 35 (U.S. GPO, Washington, D.C., 1971).

[19] J. Sugar, V. Kaufman, P. Indelicato, and W. L. Rowan, J. Opt. Soc. Am. B **6**, 1437 (1989).

[20] C. Jupén, B. Denne, and I. Martinson, Phys. Scr. **41**, 669 (1990).

[21] U. Litzén and A. Redfors, Phys. Scr. **36**, 895 (1987).

[22] J. Sugar and V. Kaufman, J. Opt. Soc. Am. B **4**, 2010 (1987).

[23] J. F. Wyart and TFR Group, Phys. Scr. **31**, 539 (1985).

[24] R. E. Stewart, D. D. Dietrich, R. J. Fortner, and R. Duckart, J. Opt. Soc. Am. B **4**, 396 (1987).

[25] J. Reader, J. Opt. Soc. Am. **73**, 796 (1983).

[26] C. Froese Fischer and M. Godefroid, Nucl. Instrum. Methods **202**, 307 (1982).

[27] D. Ray and P. K. Mukherjee, J. Phys. B **22**, 2103 (1989).

[28] K. T. Cheng and W. R. Johnson, Phys. Rev. A **16**, 263 (1977).

[29] M. Stanek, L. Glowacki, and J. Migdalek, J. Phys. B **29**, 2985 (1996).

[30] K. N. Huang and W. R. Johnson, Nucl. Instrum. Methods B **9**, 502 (1985).

[31] H. S. Chou, H. C. Chi, and K. N. Huang, J. Phys. B **26**, 4079 (1993).

[32] A. Hibbert and F. P. Keenan, J. Phys. B **20**, 4693 (1987).

[33] P. C. Ojha, F. P. Keenan, and A. Hibbert, J. Phys. B **21**, L395 (1988).

[34] C. Laughlin and G. A. Victor, Astrophys. J. **192**, 551 (1974); **234**, 407 (1979).

[35] G. A. Victor and C. Laughlin, Nucl. Instrum. Methods **110**, 189 (1973).

[36] G. A. Victor, R. F. Stewart, and C. Laughlin, Astrophys. J. Suppl. **31**, 237 (1976).

[37] J. Sucher, Phys. Rev. A **22**, 348 (1980).

[38] M. H. Mittleman, Phys. Rev. A **4**, 893 (1971); **5**, 2395 (1972); **24**, 1167 (1981).

[39] W. R. Johnson, S. A. Blundell, and J. Sapirstein, Phys. Rev. A **37**, 307 (1988).

[40] W. R. Johnson and G. Soff, At. Data Nucl. Data Tables **33**, 405 (1985).

[41] E. R. Davidson, J. Comput. Phys. **17**, 87 (1975).

[42] A. Stathopoulos and C. Froese Fischer, Comput. Phys. Commun. **79**, 268 (1994).