Relativistic calculations of $3s^2\ ^1S_0$–$3s3p\ ^1P_1$ and $3s^2\ ^1S_0$–$3s3p\ ^3P_{1,2}$ transition probabilities in the Mg isoelectronic sequence*

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Using the multi-configuration Dirac–Fock self-consistent field method and the relativistic configuration-interaction method, calculations of transition energies, oscillator strengths and rates are performed for the $3s^2\ ^1S_0$–$3s3p\ ^1P_1$ spin-allowed transition, $3s^2\ ^1S_0$–$3s3p\ ^3P_{1,2}$ intercombination and magnetic quadrupole transition in the Mg isoelectronic sequence (Mg I, Al II, Si III, P IV and S V). Electron correlations are treated adequately, including intravalence electron correlations. The influence of the Breit interaction on oscillator strengths and transition energies are investigated. Quantum electrodynamics corrections are added as corrections. The calculation results are found to be in good agreement with the experimental data and other theoretical calculations.

Keywords: transition energies, oscillator strengths, relativistic calculation, Breit interactions

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1. Introduction

Two-valence-electron atoms and ions, such as Mg I and Al II, have been chosen for many new optical clocks experiments, some of which are currently under construction and some still under consideration.[1,2] Mg-like ions are abundant in celestial objects and there are many potential lines of astrophysical interest due to the electric dipole transitions in Mg-line ions. Oscillator strengths for highly ionized atoms are still needed in astrophysics and plasma physics for diagnostic purposes. Precise calculations require various methods, including both relativistic and electron correlation effects. There are significant correlation effects between the two valence electrons and their interaction with a $n = 2$ core in Mg like ions. Our previous studies on the energy levels of a sodium-like sequence[3] and other atoms and ions[4−6] elucidated different cases about several mechanisms of anomalous fine-structure (FS) splittings.

A number of comparatively accurate experimental values[7−16], both for the allowed $3s^2{}^1S_0$–$3s3p^1P_1$ transition and for the forbidden $3s^2{}^1S_0$–$3s3p^3P_1$ transition, are available for the Mg isoelectronic sequence. The heavy-ion storage ring measurement in Al II by Träbert *et al.*[17] was carried out with an uncertainty of 3%. Theoretically, Jönsson and Fischer[18] reported transition energies and probilities using the core-valence Grasp VU multi-configuration Dirac–Fock (MCDF) package and relativistic configuration interaction (RCI) calculations that included the Breit interaction. Chou *et al.*[19] calculated excitation energies and oscillator strengths using the multi-configuration relativistic random-phase approximation, including excitation channels from core electrons. Stanek *et al.*[20] performed the calculation using the relativistic MCDF method with a polarization model to account for the valence-core electron correlation. Chen and Cheng[21] calculated the $3s^2{}^1S_0$–$3s3p^{1,3}P_1$ transition energies in Mg-like ions using the RCI method. Hibbert and Keenan[22] calculated the energies of $3s3p^{1,3}P$, $3s4s^1S$ of Al II with core polarization model potentials using the nonrelativistic con-

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figuration interaction method.

In the present paper, calculations are performed for the Mg-like sequence (Mg I, Al II, Si III, P IV and S V) using the Grasp-2K program.[23] The atomic orbitals are optimized using am MCDF self-consistent field (MCDF–SCF) calculation,[24] . Based on our former work,[25] a quasi-complete basis set can be carried out to obtain precise calculations for the transition quantities. In the RCI[26] calculations, electron correlations are adequately considered with valence–valence and core–valence electron correlations. The effects of the quantum electrodynamics (QED) corrections (the self energy and the vacuum polarization) and Breit interactions[27−29] can also be added as perturbations. Among the perturbations, the Breit interaction is the dominant correction, which represents the relativistic retardation effect of electromagnetic interactions. We perform theoretical calculations for the transition energies, oscillator strengths and rates of resonance transition $3s^2\ {}^1S_0$–$3s3p\ {}^1P_1$, the intercombination $3s^2\ {}^1S_0$–$3s3p\ {}^3P_1$ transition and magnetic quadrupole (M2) $3s^2\ {}^1S_0$–$3s3p\ {}^3P_2$ transitions.

2. Theory

In the framework of the theory of QED, in the Coulomb gauge, interactions in atomic systems can be separated into two parts: longitudinal and transverse interactions. The longitudinal interactions are instantaneous, while the transverse interactions including the interactions with radiation fields, can be treated as perturbations. For an N-electron atom or ion, the Dirac–Coulomb Hamiltonian representing instantaneous longitudinal interactions can be expressed as

$$\hat{H}_{\rm DC} = \sum_{i=1}^{N}\left[c\boldsymbol{\alpha}\cdot\boldsymbol{p}_i + (\boldsymbol{\beta}-1)c^2 - \frac{Z}{r_i}\right] + \sum_{i=1}^{N-1}\sum_{j=i+1}^{N}|\boldsymbol{r}_i-\boldsymbol{r}_j|^{-1}, \quad (1)$$

where $\boldsymbol{\alpha}_i = \begin{pmatrix} 0 & \boldsymbol{\sigma}_i \\ \boldsymbol{\sigma}_i & 0 \end{pmatrix}$, ($\boldsymbol{\sigma}_i$ is Pauli matrix, $i = 1, 2, 3$), and $\boldsymbol{\beta} = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}$. In Eq. (1), the first term is the one-body operator and the second term is the two-body Coulomb interaction between the atomic electrons. Within the average field approximation, the atomic orbital wave functions (AOs) can be obtained by numerically solving the Dirac–Fock equations self-consistently

$$\hat{H}_{\rm DC}\,|\Gamma PJM\rangle = E_\Gamma\,|\Gamma PJM\rangle\,, \quad (2)$$

where $|\Gamma PJM\rangle$ are the atomic state functions (ASFs). The ASFs are N-electron wavefunctions and can be expanded as linear combinations of configuration state functions (CSFs) with the same parity P, total angular momentum J and magnetic quantum number M,

$$|\Gamma PJM\rangle = \sum_{i=1}^{n_c} C_i^\Gamma\,|\gamma_i PJM\rangle\,, \quad (3)$$

where C^Γ are the mixing coefficients, Γ and γ represent all the other quantum numbers. The CSFs $|\gamma PJM\rangle$, which form a quasi-complete basis set in Hilbert space, are linear combinations of Slater determinants of the AOs. The AOs reveal the atomic shell structure. By applying variational method to Eq. (2), we can obtain the mixing coefficients C^Γ and the AOs self-consistently. The FS energy levels and the mixing coefficients can be obtained by diagonalizing the atomic Hamiltonian matrix.

With all the AOs of the same basis set obtained, the energy levels can be calculated using the RCI method. Thus, more atomic configurations are taken into account to adequately consider the electron correlation effects. Otherwise, more higher-order corrections are taken into account. The QED corrections (the self energy and the vacuum polarization) have little impact on the FS energy level results. The Breit interaction is the most important one out of the various corrections considered in our calculations, which can be expressed as

$$\hat{H}_{\rm T} = -\left[\frac{\boldsymbol{\alpha}_i\cdot\boldsymbol{\alpha}_j}{r_{ij}}\cos(\omega_{ij}r_{ij}) + (\boldsymbol{\alpha}_i\cdot\nabla_i)(\boldsymbol{\alpha}_j\cdot\nabla_j)\cdot\frac{\cos(\omega_{ij}r_{ij})-1}{\omega_{ij}^2 r_{ij}}\right]. \quad (4)$$

The Breit (transverse) interaction represents some high-order relativistic corrections in addition to the instantaneous Coulomb interaction, including magnetic interaction of the electron currents and the retardation effects of electromagnetic interactions with the finite velocity of light.[27−29] Although treated as secondary correction in the previous work on sodium-like sequence,[3] the Breit interaction is significant in the Mg I isoelectronic sequence.

The oscillator strength for the transition from ASF Γ_i to ASF Γ_j induced by a multipole radiation

field operator $\hat{O}_{\rm M}^{(L)}$ of order L is

$$f_{i-j} = \frac{\pi c}{(2L+1)\omega^2} \left| \left\langle \Gamma_i P_i J_i \left\| \hat{O}^{(L)} \right\| \Gamma_j P_j J_j \right\rangle \right|^2. \quad (5)$$

It can be expressed in terms of SCF matrix elements by

$$\begin{aligned} &\left| \left\langle \Gamma_i P_i J_i \left\| \hat{O}^{(L)} \right\| \Gamma_j P_j J_j \right\rangle \right| \\ &= \sum_{r,s} c_{r\Gamma_i} c_{r\Gamma_j} \left\langle \gamma_r P_r J_r \left\| \hat{O}^{(L)} \right\| \gamma_s P_s J_s \right\rangle. \end{aligned} \quad (6)$$

3. Calculation results and discussion

According to the variational principle, the present computational method is performed under the quasi-complete basis set.[25,30] The $nl(n \leq 4,\ l \leq 3)$ orbitals are referred to as spectroscopic orbitals. In order to take into account the intravalence electron correlations, we add some extra psudo-orbtials. These psudo-orbitals represent the correlations arising from the infinite bound orbitals and continuum ones approximately. These spectroscopic orbitals and psudo-orbitals can be used to form a quasi complete basis set. Using MCDF–SCF calculation, we optimize the atomic spectroscopic orbitals and the psudo-orbtials. In the RCI[26] calculations, electron correlations are adequately considered. The effects of the QED corrections (the self-energy and the vacuum polarization) and the Breit interactions[27−29] are added as perturbations. Among the perturbations, the Breit interaction is the dominant correction.[5] The $3s^2\ {}^1S_0$–$3s3p\ {}^1P_1$ allowed electric dipole (E1) transition and the $3s^2\ {}^1S_0$–$3s3p\ {}^3P_2$ magnetic quadrupole (M2) transition energies (in cm^{-1}) are shown in Table 1. Our values are compared with other theoretical results and agree well with the experimental data. The transition energies of MCDF–SCF have 2.05%–5.63% differences from the experimental data. When considering adequate electron correlation effects, the results of RCI have 0.29%–0.49% differences. The effects of the Breit interaction are added as perturbations for the results of transition energies.

Table 1. The $3s^2\ {}^1S_0$–$3s3p\ {}^1P_1$ allowed electric dipole (E1) transition and $3s^2\ {}^1S_0$–$3s3p\ {}^3P_2$ magnetic quadrupole (M2) transition energies (in cm^{-1}) in the Mg isoelectronic sequence.

	MCDF–SCF	RCI	RCI+Breit	other theory	experiments
			The $3s^2\ {}^1S_0$–$3s3p\ {}^1P_1$ transition		
Mg I	34854.053	35183.963	35181.622	35284[a)]	35051.264[31]
				35230[c)]	
				35001[d)]	
Al II	61077.942	60143.380	60137.201	60104[a)]	59852.02[32]
				59427[b)]	
				60722[c)]	
Si III	85675.279	83121.245	83113.451	83104[a)]	82884.41[33]
				82564[b)]	
				84243[c)]	
P IV	108015.286	105506.278	105496.698	105398[a)]	105190.42[34]
S V	130549.169	127533.263	127522.082	127350[a)]	127150.7[35]
				127403[b)]	
				129272[c)]	
			$3s^2\ {}^1S_0$–$3s3p\ {}^3P_2$		
Mg I	15406.512	21934.927	21932.674	21721[a)]	21911.178[31]
Al II	29498.141	37573.319	37567.202	37376[a)]	37577.79[32]
Si III	43926.587	53197.403	53187.789	52867[a)]	53115.01[33]
P IV	58506.278	68674.950	68660.474	68347[a)]	68615.17[34]
S V	73223.797	84168.615	84148.470		84155.2[35]

[a)] The values are from core-valence calculations including the Breit interaction by Jönsson and Fischer.[18]

[b)] Calculation including three configurations and without core excitation channels, which is the best result from Chou *et al.*[19]

[c)] Stanek *et al.*[20]

[d)] Chen and Cheng.[21]

Table 2 shows the calculation results of the $3s^2\ {}^1S_0$–$3s3p\ {}^3P_1$ intercombination (IC) transition energies and

rates. The FS splittings for 3s3p ^{3}P agree well with the experimental data. Within the relativistic framework, transition matrix elements may be calculated in different gauges. For electric transitions, both the Babushkin and Coulomb gauges can be used. The former is more sensitive to the other part of the wavefunctions and approaches the length form in the non-relativistic limit. The latter investigates more of the inner parts and approaches the velocity form. For approximate relativistic wavefunctions, the values of the matrix elements in the two gauges will differ. The Babushkin gauge generally provides the most reliable values at a given level of valence and core-valence electron correlation. This is particularly true for IC transitions where the dependence on the gauge is particularly strong. The present calculations on transition rates are shown in the Babushkin gauge. Based on the quasi basis set, the IC rates are taken from the preceding calculation. The Breit interactions on transition rates and oscillator strength are further elucidated in Tables 3 and 4.

Table 2. Fine structure splittings for 3s3p ^{3}P and transition energies ΔE and rates A for the 3s^2 ^{1}S$_0$–3s3p ^{3}P$_1$ IC lines in the Mg isoelectronic sequence.

	$\Delta E^{\rm fs}_{1-0}$/cm^{-1}	$\Delta E^{\rm fs}_{2-1}$/cm^{-1}	$\Delta E_{\rm IC}$/cm^{-1}	$A^{\rm B}_{\rm IC}$/s^{-1}
			Mg I	
RCI+Breit	19.791	40.194	21892.480	208.3
theories	19.83[a)]	40.06[a)]	21681[a)]	197.3[a)]
			21835[d)]	175[b)]
				172[c)]
experiments	20.419[31]	40.714[31]	21870.464[31]	196(23)[36]
			Al II	
RCI+Breit	60.471	123.121	37444.081	3775.063
theories	60.5[a)]	123.2[a)]	37253[a)]	2979[a)]
			36332[b)]	2719[b)]
			37393[e)]	2496[c)]
			36562[f)]	3500[h)]
			38006[g)]	
experiments	60.9[32]	123.9[32]	37453.91[32]	3280±100[17]
				3330±230[37]
			Si III	
RCI+Breit	129.5	264.732	52884.818	18287
theories	127.6[a)]	260.8[a)]	52606[a)]	16133[a)]
				15369[b)]
				13814[c)]
				16700[i)]
experiments	128[33]	261[33]	52853.28[33]	16700±500[38]
			P IV	
RCI+Breit	227.250	467.147	68193.327	62627.2
theories	227.4[a)]	467.5[a)]	67879[a)]	57237[a)]
				55691[b)]
				49498[c)]
experiments	227.4[34]	468.4[34]	68146.48[34]	–
			S V	
RCI+Breit	367.275	760.056	83388.413	165287.0
experiments	369.5[35]	761.7[35]	83393.5[36]	–

Superscripts B denotes the Babushkin gauge.

a) The values are spd limit corrected for fgh contributions by Jönsson and Fischer.[18]

b) The values of the MCRRPA calculations by Chou *et al.*[19]

c) The values from the Model potential MCDF-CP calculations by Stanek *et al.*[20]

d) Chen and Cheng.[21]

e) Angstmann *et al.*[39]

f) The calculations including three configurations and without core excitation channels, Hibbert and Keenan (1987).[22]

g) Calculation including five configurations and without core excitation channels, Hibbert and Keenan (1987).[22]

h) CIV3.[40] i) CIV3.[41]

The weighted oscillator strengths for the spin-allowed and spin-forbidden transitions are shown in Table 3. Our RCI results based on the quasi basis set are in good agreement with the experimental data and other theoretical results. The transition energies in the Mg isoelectronic sequence are mainly affected by the electron correlation effects, as shown in Table 1. The Breit interaction has less impact on transition energies and the oscillator strengths of the spin-allowed transition. However, the Breit interaction is very important for the spin-forbidden transitions, as shown in oscillator results in Table 3 and the 3s3p ^{3}P FS splittings and the intercombination rate in Table 4.

Table 3. Oscillator strengths of the spin-allowed $3s^2\ ^1S_0$–$3s3p\ ^1P_1$ transition and the spin-forbidden $3s^2\ ^1S_0$–$3s3p\ ^3P_1$ transition in the Mg isoelectronic sequence.

	$3s^2\ ^1S_0$–$3s3p\ ^1P_1$ transition				
methods	Mg I	Al II	Si III	P IV	S V
RCI+Breit	1.722	1.785	1.646	1.507	1.390
RCI	1.721	1.785	1.646	1.507	1.390
theories	1.709[a)]	1.751[a)]	1.611[a)]	1.477[a)]	1.360[a)]
	1.72[c)]	1.779[b)]	1.647[b)]	1.516[b)]	1.402[b)]
		1.77[c)]	1.62[c)]	1.49[c)]	1.37[c)]
exp.	1.75(9)[A)]	1.74(27)[C)]	1.64(24)[D)]	1.85(17)[F)]	1.46(8)[H)]
	1.83(9)[B)]		1.60(35)[E)]	1.16(7)[G)]	1.06(8)[I)]
					0.99(3)[J)]
	$3s^2\ ^1S_0$–$3s3p\ ^3P_1$ transition				
methods	Mg I	Al II	Si III	P IV	S V
RCI+Breit	1.99(–6)	1.21(–5)	2.936(–5)	6.06(–5)	1.07(–4)
RCI	2.28(–6)	1.35(–5)	3.257(–5)	6.67(–5)	1.71(–4)
theories	1.802(–6)[b)]	9.284(–6)[b)]	2.587(–5)[b)]	5.568(–5)[b)]	1.038(–4)[b)]
	1.705(–6)[c)]	8.333(–6)[c)]	2.299(–5)[c)]	4.931(–5)[c)]	9.193(–5)[c)]
exp.	(2.50±0.80)(–6)[B)]	(1.068±0.074)(–5)[E)]	(2.67±0.16)(–5)[F)]	(2.70±0.16)(–5)[C)]	
	(2.06±0.29)(–6)[C)]				
	(1.84±0.20)(–6)[D)]				

a) The values from the core-valence calculation by Jönsson and Fischer.[18]
b) The values from the Model potential MCDF-CP calculations by Stanek *et al.*[20]
c) The values from the MCRRPA calculations by Chou *et al.*[19]
[A)] Beam-foil, Lundin.[7]
[B)] Beam-foil, Liljeby *et al.*[8]
[C)] Beam-foil, Kernahan *et al.*[9]
[D)] Beam-foil, Irwin and Livingston.[11]
[E)] Beam-foil, Livingston.[12]
[F)] Beam-foil, Curtis *et al.*[12]
[G)] Beam-foil, Livingston *et al.*[13]
[H)] Beam-foil, ANDC corrected, Reistad *et al.*[14]
[I)] Beam-foil, Irwin and Livingston.[15]
[J)] Beam-foil, Dumont *et al.*[16]

In Table 4, we compare the calculation results for the FS splitting of 3s3p ^{3}P and transition rates with and without the Breit interaction. The Breit interaction has the same impact on the FS splitting as the results from Jönsson and Fischer.[18] The influence on transition rates are in the same sides. It is seen that the effect of the Breit interaction is to decrease both FS splitting and the IC rate. Considering the Breit interaction, including magnetic interaction of electron currents and the retardation effects of electromagnetic interactions with the finite velocity of light,[27−29] we find that the transition rates are becoming smaller.

Table 4. Effect of the Breit interaction for the FS splittings of 3s3p ^{3}P and the transition energies and rates for the the 3s^2 ^{1}S$_0$–3s3p ^{3}P$_1$ IC of Mg I.

	$\Delta E^{\rm fs}_{1-0}$/cm^{-1}	$\Delta E^{\rm fs}_{2-1}$/cm^{-1}	$\Delta E_{\rm IC}$/cm^{-1}	$A^{\rm B}_{\rm IC}$/s^{-1}
	without the Breit interaction			
RCI	21.613	43.336	21891.591	238.7
Jönsson and Fischer[18]	20.48	41.04	21030	192.6
	with the Breit interaction			
RCI	19.791	40.194	21892.480	208.3
Jönsson[18]	19.23	38.80	21029	175.7
experiments	20.419	40.714	21870.464	196.23[42]

4. Conclusion

Precise theoretical calculations are performed on the FS energy levels in a Mg isoelectronic sequence. The good agreement with the experimental data illustrates the validity of the present quasi complete basis set construction. The computational method is feasible for energy levels of every excited state and different atoms or ions. Due to the full relativistic theoretical systems, the computational method is also viable for theoretical studies on high Z atoms and high ionization ions. Based on the precise energy levels, many physical quantities (i.e. hyperfine structures) could be studied.

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