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Transition properties of the Be-like Kα X-ray from Mg IX

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Abstract. Energy levels among the lowest 40 fine-structure levels in Be-like Mg IX are calculated using grasp2K code. The wavelengths, oscillator strengths, radiative rates and lifetimes for all possible Kα transitions have been calculated using the multiconfiguration Dirac–Fock method. The accuracy of the results is determined through extensive comparisons with the existing laboratory measurements and theoretical results. The present data can be used reliably for many purposes, such as the line identification of the observed spectra, and modelling and diagnostics of magnesium plasma.

Keywords. Energy levels; radiative rates; transition probabilities.

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1. Introduction

Magnesium is one of the most abundant elements in the Universe, and its spectral lines at various stages have been commonly observed in a host of different astrophysical objects [1]. Mg IX is formed in the temperature range of $5 \times 10^5 - 8 \times 10^6$ K and its strongest line at 367.07 Å can be used to measure emission of the coronal plasma in the solar and stellar coronae [2]. Intensity ratio between Mg IX lines can be used to measure the electron density and the electron temperature in quiet plasma. Ratios with lines emitted from ions of other elements formed at similar temperatures can be used to infer the relative abundance of Mg compared to these elements. Mg can be a trace layer buried in an ablator, line ratios and line intensities represent the ionization balance [3]. Mg Kα lines typically contain contributions from different charge states, and their analyses provide useful information about the equilibrium and non-equilibrium charge-state distributions of ions [4].

In view of this importance of Mg Kα line for astrophysics and laboratory diagnostics, accurate theoretical predictions are needed for the reliable identification and interpretation of experimental spectral data [4]. The simplest ion contributing to the Kα line is the helium-like ion. Be-like Mg IX is the complex four-electron, and more complex Kα lines such as Li-like and Be-like should be considered. In view of this situation, the importance of Be-like transitions of Kα have been long recognized, and several studies have been devoted to the prediction of energies, wavelengths and radiative rates. Energies of the ten states of Mg IX were determined with second order in relativistic many-body perturbation by Safronova *et al* [5]. The energy levels and oscillator strengths of Be-like ions for Z = 5–14 were calculated by Kingston and Hibbert [6] using the Breit–Pauli (BP) method. The fine structure energies of low-lying excited states of Mg IX were calculated with multiconfiguration interaction method and restricted variation method (RVM) by Han *et al* [7]. Kα X-ray satellites of magnesium ions (including Mg IX) were calculated by Deng *et al* with relativistic configuration interaction [8].

However, at present, experimental and theoretical data on these systems are not sufficiently complete. Only two Kα transitions of Be-like were considered in [8], and complete transitions for $1s^2 2s2p$–$1s2s2p^2$ were not given in [7]. Hu *et al* have made a model for laser-produced plasma, and found that Kα transitions from

Be-like ions have an important influence on the temperature and density of ions [9]. In the present work, energy levels and radiative data of Kα transition in Be-like Mg IX are discussed in the framework of relativistic configuration interaction (RCI) formalism by using multiconfiguration Dirac–Fock (MCDF) wave functions. Breit interaction and quantum electrodynamics (QED) were considered in the calculations. These calculations are performed using the general purpose relativistic atomic structure package (grasp2K) [10,11]. It is a modification and extension of the GRASP92 package by Parpia *et al* [12].

2. Method

2.1 *MCDF*

In the MCDF approach, the wave function for a state labelled γJ, where γ represents the configuration and any other quantum numbers required to specify the state, is approximated by an expansion over *jj*-coupled configuration state functions (CSFs)

$$\Psi(\gamma J) = \sum_i C_i \Phi_i(\gamma_i J). \tag{1}$$

The configuration state functions $\Psi(\gamma J)$ are antisymmetrized linear combinations of products of relativistic orbitals

$$\Phi(r) = \frac{1}{r}\begin{pmatrix} P_{n\kappa}(r)\chi_{\kappa m}(\vec{r}) \\ iQ_{n\kappa}(r)\chi_{-\kappa m}(\vec{r}) \end{pmatrix}. \tag{2}$$

Here κ is the relativistic angular momentum, $P_{n\kappa}(r)$ and $Q_{n\kappa}(r)$ are the large and small components of radial wave functions, respectively and $\chi_{\kappa m}(\vec{r})$ is the spinor spherical harmonic in the *lsj* couping scheme.

$$\chi_{\kappa m}(\vec{r}) = \sum_{m_l, m_s} \left\langle l\frac{1}{2}m_l m_s \middle| jm \right\rangle Y_{lm_l}(\theta, \varphi)\xi_{m_s}(\sigma). \tag{3}$$

The radial functions $P_{n\kappa}(r)$ and $Q_{n\kappa}(r)$ are numerically represented on a logarithmic grid and are required to be orthonormal within each κ symmetry

$$\int_0^\infty [P_{n'\kappa}(r)P_{n\kappa}(r) + Q_{n'\kappa}(r)Q_{n\kappa}(r)]\mathrm{d}r = \delta_{n'n}. \tag{4}$$

In the multiconfiguration self-consistent field (MCSCF) procedure both the radial functions and the expansion coefficients for the configuration state functions are optimized to self-consistency [12].

2.2 *RCI*

Once a set of radial orbitals has been obtained, RCI calculations can be performed. Here only the expansion coefficients of the CSFs are determined. This is achieved by diagonalizing the Hamiltonian matrix. In this implementation of the RCI program, the iterative Davidson method is used together with a sparse matrix representation allowing for large expansions.

In the RCI calculations, the transverse photon interaction may be included in the Hamiltonian

$$H_{\mathrm{trans}} = -\sum_{i<j}\left[\frac{\alpha_{\mathbf{i}}\cdot\alpha_{\mathbf{j}}}{R_{ij}} + (\alpha_{\mathbf{i}}\cdot\nabla_{\mathbf{i}})(\alpha_{\mathbf{j}}\cdot\nabla_{\mathbf{j}})\frac{\cos\omega_{ij}R_{ij}}{\omega_{ij}^2 R_{ij}}\right], \tag{5}$$

where photon frequency ω_{ij} used by the RCI program in calculating the matrix elements of the transverse photon interaction is taken to be the difference in the diagonal Lagrange multipliers and associated with the orbitals. In general, diagonal Lagrange multipliers are approximate electron removal energies only when orbitals are spectroscopic and singly occupied. Thus, it is not known how well the code can determine the full transverse photon interaction when correlation orbitals are present. What can be obtained instead is the low frequency limit $\omega_{ij} \to 0$ usually referred to as the Breit interaction.

2.3 *QED*

There are two major components in the QED correction [13]. Known simply as self-energy, the dominant correction to energy arises from the lowest-order modification to an electron's interaction with quantized ambient electromagnetic field when in the presence of the field due to the nucleus and the other atomic electrons. In terms of a function $F_{n\kappa}^{\mathrm{SE}}$ that varies slowly with respect to its argument, the self-energy in hydrogen-like systems is given by

$$F_{n\kappa}^{\mathrm{SE}}(Z/c) = \frac{Z^4}{\pi c^3 n^3}F_{n\kappa}(Z/c). \tag{6}$$

Tabulations of $F_{n\kappa}(Z/c)$ for the 1s, 2s, $2p_{1/2}$, and $2p_{3/2}$ states in these one-electron systems are given in refs [14] and [15]. In grasp2K a rough estimate of the self-energy is obtained by setting

$$E_{n_a\kappa_a}^{\mathrm{SE}} = \frac{(Z_a^{\mathrm{eff}})^4}{\pi c^3 n^3} \times \begin{cases} F_{n_a\kappa_a}(Z_a^{\mathrm{eff}}/c), & \text{for } n = 1, 2 \text{ orbitals}, \\ F_{2\kappa_a}(Z_a^{\mathrm{eff}}/c), & \text{for } n(\geq 3) \text{ orbitals}, \\ 0, & \text{otherwise}. \end{cases}$$

The use of Z^{eff} to roughly correct for electron screening is at best an expedient intended for inner shells where the orbitals are most likely to be nearly hydrogenic. It is likely to be increasingly less realistic as n increases.

Next in the order of importance is, the vacuum polarization correction. To lowest order, this is the short-range modification of the nuclear field due to screening by virtual electron–positron pairs. Expression for the second- and fourth-order perturbation potentials that take fine nuclear size into account have been given in the literature, for example in ref. [16]. Only diagonal contributions,

$$H_{rr}^{\text{VP}} = \sum_{a=1}^{n_w} q_r(a) \int_0^\infty \mathrm{d}r\, V^{\text{VP}}(r)(P^2_{n_a\kappa_a}(r) + Q^2_{n_a\kappa_a}(r)) \tag{7}$$

from these potentials have been included in this version of grasp2K.

Table 1. Energy levels (in eV) of Be-like Mg IX. $a(b) \equiv a \times 10^b$.

Key	Configuration	Term	Breit	VP	SE	Total	NIST
1	$1s^2 2s^2$	$^1S_0$				0.0000	0.0000
2	$1s^2 2s2p$	$^3P^o_0$	4.2207(−2)	1.4562(−3)	−2.1392(−2)	1.7434(1)	1.7420(1)
3		$^3P^o_1$	1.8351(−2)	1.4568(−3)	−2.1021(−2)	1.7571(1)	1.7560(1)
4		$^3P^o_2$	−1.1602(−2)	1.4582(−3)	−2.2238(−2)	1.7871(1)	1.7865(1)
5		$^1P^o_1$	4.5131(−3)	1.4640(−3)	−2.2717(−2)	3.3635(1)	3.3684(1)
6	$1s^2 2p^2$	$^3P_0$	5.1272(−2)	3.1076(−3)	−5.1338(−2)	4.5344(1)	4.5360(1)
7		$^3P_1$	3.8133(−2)	3.1085(−3)	−5.0911(−2)	4.5501(1)	4.5522(1)
8		$^3P_2$	−8.7433(−3)	3.1098(−3)	−5.1186(−2)	4.5764(1)	4.5791(1)
9		$^1D_2$	5.3897(−3)	3.1052(−3)	−5.1414(−2)	5.0294(1)	5.0226(1)
10		$^1S_2$	3.9306(−2)	2.9142(−3)	−4.9183(−2)	6.3093(1)	6.1947(1)
11	$1s2s^2 3p$	$^3P^o_0$	−4.6420(−1)	1.6574(−2)	−2.6897(−1)	1.3136(3)	
12		$^3P^o_1$	−5.6846(−1)	1.6576(−2)	−2.6867(−1)	1.3137(3)	
13		$^3P^o_2$	−6.0998(−1)	1.6580(−2)	−2.6795(−1)	1.3141(3)	
14		$^1P^o_1$	−6.3128(−1)	1.6577(−2)	−2.6824(−1)	1.3220(3)	1.3214(3)
15	$1s2s2p^2$	$(^3S^3P)^5P_1$	−5.3617(−1)	1.8040(−2)	−2.9361(−1)	1.3167(3)	
16		$(^3S^3P)^5P_2$	−5.4257(−1)	1.8041(−2)	−2.9321(−1)	1.3169(3)	
17		$(^3S^3P)^5P_4$	−6.3780(−1)	1.8042(−2)	−2.9264(−1)	1.3171(3)	
18		$(^1S^3P)^3P_0$	−6.1308(−1)	1.8038(−2)	−2.9361(−1)	1.3352(3)	1.3347(3)
19		$(^1S^3P)^3P_1$	−6.0860(−1)	1.8039(−2)	−2.9338(−1)	1.3353(3)	1.3349(3)
20		$(^1S^3P)^3P_2$	−6.0128(−1)	1.8040(−2)	−2.9307(−1)	1.3355(3)	1.3352(3)
21		$(^3S^1D)^3D_3$	−6.8010(−1)	1.8041(−2)	−2.9299(−1)	1.3357(3)	1.3344(3)
22		$(^3S^1D)^3D_1$	−5.2492(−1)	1.8041(−2)	−2.9294(−1)	1.3359(3)	1.3346(3)
23		$(^3S^1D)^3D_2$	−5.9589(−1)	1.8041(−2)	−2.9264(−1)	1.3359(3)	1.3346(3)
24		$(^3S^1S)^3S_1$	−5.8010(−1)	1.8041(−2)	−2.9303(−1)	1.3445(3)	
25		$(^1S^1D)^1D_2$	−5.3416(−1)	1.8040(−2)	−2.9305(−1)	1.3477(3)	1.3460(3)
26		$(^3S^3P)^3P_0$	−4.8983(−1)	1.8040(−2)	−2.9364(−1)	1.3489(3)	
27		$(^3S^3P)^3P_1$	−4.8922(−1)	1.8041(−2)	−2.9325(−1)	1.3492(3)	
28		$(^3S^3P)^3P_2$	−5.7884(−1)	1.8042(−2)	−2.9263(−1)	1.3494(3)	1.3472(3)
29		$(^3S^3P)^1P_1$	−6.6167(−1)	1.8041(−2)	−2.9296(−1)	1.3558(3)	1.3537(3)
30		$(^1S^1S)^1S_0$	−4.8426(−1)	1.8039(−2)	−2.9287(−1)	1.3566(3)	
31	$1s2p^3$	$^5S_2$	−5.3416(−1)	1.9692(−2)	−3.2093(−1)	1.3464(3)	
32		$^3D_1$	−6.5176(−1)	1.9693(−2)	−3.2091(−1)	1.3591(3)	1.3576(3)
33		$^3D_2$	−5.0358(−1)	1.9692(−2)	−3.2095(−1)	1.3592(3)	1.3577(3)
34		$^3D_3$	−4.9321(−1)	1.9692(−2)	−3.2096(−1)	1.3592(3)	1.3577(3)
35		$^3S_1$	−6.4686(−1)	1.9692(−2)	−3.2096(−1)	1.3624(3)	
36		$^1D_2$	−6.1881(−1)	1.9680(−2)	−3.2095(−1)	1.3671(3)	1.3650(3)
37		$^3P_0$	−6.4499(−1)	1.9506(−2)	−3.1771(−1)	1.3682(3)	
38		$^3P_1$	−4.3977(−1)	1.9515(−2)	−3.1757(−1)	1.3682(3)	
39		$^3P_2$	−4.6580(−1)	1.9506(−2)	−3.1781(−1)	1.3682(3)	1.3664(3)
40		$^1P_1$	−6.0062(−1)	1.9504(−2)	−3.1767(−1)	1.3762(3)	1.3739(3)

Table 2. Energy level (in eV) of $1s^2 2s2p$ and $1s^2 2p^2$ obtained by different methods.

Method	$2s2p\ ^3P_0$	$2s2p\ ^3P_1$	$2s2p\ ^3P_2$	$2p^2\ ^3P_0$	$2p^2\ ^3P_1$	$2p^2\ ^3P_2$
MCDF[a]	1.7434(1)	1.7571(1)	1.7871(1)	4.5344(1)	4.5501(1)	4.5764(1)
RVM[b]	1.7470(1)	1.7613(1)	1.7913(1)	4.5473(1)	4.5623(1)	4.5901(1)
BP[c]	1.7498(1)	1.7635(1)	1.7937(1)	4.5602(1)	4.5760(1)	4.6025(1)
MBPT[d]	1.7412(1)	1.7552(1)	1.7857(1)	4.5347(1)	4.5509(1)	4.5779(1)
Exp[e]	1.7420(1)	1.7560(1)	1.7865(1)	4.5360(1)	4.5526(1)	4.5791(1)

[a]This work.
[b]Han *et al* [7].
[c]Kingston and Hibbert [6].
[d]Safronova *et al* [5].
[e]Kramida *et al* [18].

Table 3. Comparison of the calculated term energies (in eV) of $1s2s2p^2$.

Term	NIST	MCDF[a]	MCDF[b]	RMBPT[c]
$(^3S^3P)^5P_1$		1.3167(3)	1.3148(3)	1.3173(3)
$(^3S^3P)^5P_2$		1.3169(3)	1.3151(3)	1.3176(3)
$(^3S^3P)^5P_3$		1.3171(3)	1.3154(3)	1.3176(3)
$(^3S^3P)^3P_0$	1.3347(3)	1.3352(3)	1.3334(3)	1.3352(3)
$(^3S^3P)^3P_1$	1.3349(3)	1.3353(3)	1.3336(3)	1.3352(3)
$(^3S^3P)^3P_2$	1.3352(3)	1.3355(3)	1.3341(3)	1.3355(3)
$(^3S^1D)^3D_3$	1.3344(3)	1.3357(3)	1.3336(3)	1.3350(3)
$(^3S^1D)^3D_1$	1.3346(3)	1.3359(3)	1.3339(3)	1.3350(3)
$(^3S^1D)^3D_2$	1.3346(3)	1.3359(3)	1.3339(3)	1.3350(3)
$(^3S^1S)^3S_1$		1.3445(3)	1.3429(3)	1.3440(3)
$(^1S^1D)^1D_2$	1.3460(3)	1.3477(3)	1.3459(3)	1.3464(3)
$(^1S^3P)^3P_0$		1.3489(3)	1.3450(3)	1.3472(3)
$(^1S^3P)^3P_1$		1.3492(3)	1.3469(3)	1.3472(3)
$(^1S^3P)^3P_2$	1.3472(3)	1.3494(3)	1.3472(3)	1.3475(3)
$(^1S^3P)^1P_1$	1.3537(3)	1.3558(3)	1.3540(3)	1.3537(3)
$(^1S^1S)^1S_0$		1.3566(3)	1.3540(3)	1.3554(3)

[a]This work.
[b]Sang *et al* [19].
[c]Safronova *et al* [5].

Table 4. Wavelength (in nm) of Kα transitions of Be-like Mg.

I	J	Exp[a]	Fit[a]	Int[a]	Present	Diff[b]
9	40		9.3670	14	9.3609	0.0061
1	14	9.3840	9.3830	43*bl**	9.3782	0.0048
8	39	9.3840	9.3885	43*bl**	9.3745	0.0014
5	29	9.3930	9.3930	49	9.3864	0.0066
4	28	9.4410	9.4112	86*bl**	9.4064	0.0048
2	22	9.4410	9.4126	*	9.4051	0.0075
3	18	9.4410	9.4127	*	9.4114	0.0013
3	23	9.4410	9.4141	*	9.4060	0.0081
4	21	9.4300	9.4168	32*bl**	9.4094	0.0074
9	36	9.4300	9.4303	32*bl**	9.4255	0.0048
6	32	9.4300	9.4475	32*bl**	9.4360	0.0115
5	25	9.4300	9.4477	32*bl**	9.44485	0.0029
7	33	9.4300	9.4487	32*bl**	9.4428	0.0059
10	40	9.4540	9.4510	25*bl**	9.4494	0.0016
8	34	9.4540	9.4516	25*bl**	9.4392	0.0124

[a]Boiko *et al* [20].
[b]Fit-present.
bl – Blended with another line.
*Intensity is shared by several lines.

2.4 *Calculation procedure*

First, MCDF calculations in the extended optimal level (EOL) scheme were performed for each group of atomic states. Configuration expansions including all lower states of the same J symmetry and parity, and a Dirac–Coulomb version were used. Secondly, orbitals including Breit corrections were optimized in a final configuration interaction calculation.

To build a CSF expansion, the restrictive active space method was also used. That is, consider only electrons from the active space and excite them from the occupied orbitals to the unoccupied ones. In order to monitor the convergence of the calculation, the orbital should be increased systematically. With the same principal quantum number n, the orbitals often have similar energies. The active set is usually enlarged in steps of orbital layers. It is convenient to refer to the {1s, 2s, 2p} set of orbitals as the $n = 2$ orbital layer, {1s, 2s, 2p, 3s, 3p, 3d} as the $n = 3$ layer, etc. Larger orbital sets can result in a considerable increase of computational time required for the problem, and appropriate restrictions may be necessary. We divided up the calculations into two parts, one where we optimized a set of orbitals for the even states and one for the odd states, i.e. the upper and lower states were described by two independently optimized sets of orbitals. Because of this, we had to use biorthogonal transformation [17] of the atomic state functions to calculate the transition parameters. Only the newly added orbitals were optimized to reduce the processing time. So for Be-like Mg IX, the active set (AS)

$$\mathrm{AS1} = \{3s, 3p, 3d\}. \tag{8}$$

Table 5. Wavelengths (in nm), transition probabilities (in s^{-1}) and oscillator strengths of Be-like Mg.

I	J	λ	A_v	A_l	f_v	f_l	dT[a]
1	12	9.4378	2.4384(10)	2.5488(10)	9.7680(−4)	1.0210(−3)	0.0433
1	14	9.3782	1.6524(13)	1.7240(13)	6.5361(−1)	6.8192(−1)	0.0415
2	19	9.4094	1.0584(13)	1.1170(13)	4.2142(−1)	4.4476(−1)	0.0525
2	22	9.4051	2.2788(12)	2.2440(12)	9.0654(−2)	8.9272(−2)	0.0153
2	24	9.3435	8.7313(11)	9.3933(11)	3.4281(−2)	3.6880(−2)	0.0705
2	27	9.3113	3.0441(11)	2.9872(11)	1.1870(−2)	1.1648(−2)	0.0187
3	18	9.4114	2.4095(13)	2.5623(13)	3.1994(−1)	3.4023(−1)	0.0596
3	19	9.4104	4.1606(12)	4.4724(12)	1.6570(−1)	1.7812(−1)	0.0697
3	20	9.4087	1.1622(13)	1.2104(13)	7.7116(−1)	8.0314(−1)	0.0398
3	22	9.4061	5.5569(12)	5.6670(12)	2.2111(−1)	2.2549(−1)	0.0194
3	23	9.4060	7.8440(11)	7.2856(11)	5.2018(−2)	4.8315(−2)	0.0712
3	24	9.3445	2.7155(12)	2.9249(12)	1.0664(−1)	1.1486(−1)	0.0716
3	26	9.3135	1.1866(12)	1.1757(12)	1.5430(−2)	1.5289(−2)	0.0092
3	27	9.3123	2.1373(11)	2.0821(11)	8.3359(−3)	8.1202(−3)	0.0258
3	28	9.3107	2.2964(11)	2.2633(11)	1.4921(−2)	1.4707(−2)	0.0144
4	19	9.4126	8.6896(12)	9.2543(12)	3.4623(−1)	3.6874(−1)	0.0610
4	20	9.4108	8.4160(12)	9.0712(12)	5.5868(−1)	6.0218(−1)	0.0722
4	21	9.4094	8.4484(12)	8.5062(12)	7.8494(−1)	7.9031(−1)	0.0068
4	22	9.4082	1.2778(12)	1.3286(12)	5.0865(−2)	5.2890(−2)	0.0382
4	23	9.4081	1.1795(13)	1.2303(13)	7.8258(−1)	8.1627(−1)	0.0413
4	24	9.3466	4.8466(12)	5.2311(12)	1.9041(−1)	2.0552(−1)	0.0735
4	25	9.3250	3.3381(10)	3.3966(10)	2.1757(−3)	2.2139(−3)	0.0172
4	27	9.3144	6.5494(11)	6.5642(11)	2.5555(−2)	2.5612(−2)	0.0023
4	28	9.3128	8.1283(11)	8.0226(11)	5.2840(−2)	5.2153(−2)	0.0130
5	25	9.4448	8.2517(12)	8.5581(12)	5.5174(−1)	5.7423(−1)	0.0358
5	26	9.4352	2.6923(10)	2.9411(10)	3.5930(−4)	3.9251(−4)	0.0846
5	27	9.4339	2.6923(10)	2.9411(10)	3.5930(−4)	3.9251(−4)	0.0492
5	28	9.4322	1.0043(11)	1.0469(11)	6.6973(−3)	6.9812(−3)	0.0407
5	29	9.3864	2.5209(13)	2.6445(13)	9.9888(−1)	1.0479(−0)	0.0467
5	30	9.3811	8.3580(12)	9.2680(12)	1.1027(−1)	1.2227(−1)	0.0982
6	34	9.4417	4.8654(12)	4.9021(12)	1.9506(−1)	1.9653(−1)	0.0075
6	35	9.4187	3.9344(12)	4.2075(12)	1.5697(−1)	1.6787(−1)	0.0649
6	37	9.3777	2.2418(12)	2.3543(12)	8.8664(−2)	9.3114(−2)	0.0478
7	33	9.4428	6.5490(12)	6.5964(12)	4.3771(−1)	4.7088(−1)	0.0072
7	34	9.4428	3.3212(12)	3.3398(12)	1.3318(−1)	1.3393(−1)	0.0056
7	35	9.4198	1.1576(13)	1.2377(13)	4.6197(−1)	4.9395(−1)	0.0647
7	36	9.3862	9.4433(10)	9.9515(10)	6.2361(−3)	6.5718(−3)	0.0511
7	37	9.3789	1.7798(12)	1.8621(12)	7.0409(−2)	7.3667(−2)	0.0442
7	38	9.3784	1.6464(12)	1.7323(13)	1.0854(−1)	1.1421(−1)	0.0496
7	39	9.3784	7.9498(12)	8.3451(12)	1.0482(−1)	1.1003(−1)	0.0474
8	32	9.4457	8.3990(12)	8.4515(12)	7.8637(−1)	7.9129(−1)	0.0062
8	33	9.4447	1.8373(12)	1.8446(12)	1.2285(−1)	1.2332(−1)	0.0040
8	34	9.4447	1.9762(11)	1.9842(11)	7.9283(−3)	7.9603(−3)	0.0040
8	35	9.4217	1.8067(13)	1.9327(13)	7.2129(−1)	7.7156(−1)	0.0652
8	36	9.3881	6.6730(11)	7.0019(11)	4.4085(−2)	4.6258(−2)	0.0470
8	37	9.3807	3.9611(12)	4.1635(12)	1.5676(−1)	1.6478(−1)	0.0486
8	38	9.3802	5.5820(12)	5.8535(12)	3.6816(−1)	3.8606(−1)	0.0464
9	32	9.4834	1.4520(10)	1.4535(10)	1.3704(−3)	1.3718(−3)	0.0010
9	38	9.4176	1.7689(12)	1.8555(12)	1.1759(−1)	1.2335(−1)	0.0467
9	40	9.3609	1.3226(13)	1.4446(13)	5.2123(−1)	5.6930(−1)	0.0844
10	40	9.4494	1.1420(13)	1.1749(13)	4.5860(−1)	4.7182(−1)	0.0280

[a] $dT = \mathrm{abs}(A_l - A_v)/\max(A_l, A_v)$.

Then, we increase the AS in the way shown as follows:

$$\mathrm{AS2} = \mathrm{AS1} + \{4s, 4p, 4d, 4f\}, \quad (9)$$

$$\mathrm{AS3} = \mathrm{AS2} + \{5s, 5p, 5d, 5f\}, \quad (10)$$

$$\mathrm{AS4} = \mathrm{AS3} + \{6s, 6p, 6d, 6f\}. \quad (11)$$

The largest AS included relativistic orbitals with $n \leq 6$ and $l \leq 3$. We limited our orbital set to $l \leq 3$ as results converged reasonably and no significant difference was noticed in the results with $l \geq 3$. This will be found in the discussion.

3. Results and discussion

Results for $1s^22s^2$, $1s^22s2p$, $1s^22p^2$, $1s2s^22p$, $1s2s2p^2$ and $1s2p^3$ levels are displayed in descending order in table 1. The values in the column labelled Exp. in table 1 are obtained from the National Institute of Standards and Technology (NIST) by Kramida *et al* [18]. Contribution from Breit, vacuum polarization and self-energy are considered. Self-energy is found to be the major contributor of QED as shown in [8,13]. Vacuum polarization and self-energy are found to be of the same order for all transitions considered in this work. The largest discrepancy between our computed energies and NIST values is less than 0.22%.

In order to check the reliability of our calculation, comparison for energy levels of $1s^22s2p$ and $1s^22p^2$ are shown in table 2. Also included in this table are values obtained by Han *et al* [7], who adopted Rayleigh–Ritz method (RRM) and energies from Kingston and Hibbert [6] who used BP method, and the data from Safronova *et al* [5] by using the relativistic many-body perturbation (RMBPT) theory. The present results agree well with NIST, and much better than results from RRM and BP. Compared to the RMBPT, ours are little higher with the range of 3–22 eV. Also, results for $1s2s2p^2$ have been given in table 3, calculation have been done by Sang *et al* [19] by using the computational program GRASP92 based on the MCDF method, and Safronova *et al* [5] had done an earlier work with RMBPT method. Differences between our results for $1s2s2p^2$ and those of NIST are in range of 3–22 eV and differences are in the range of 14–23 eV between our results and those of Sang *et al* [19]. Ours are generally in agreement with Safronova *et al* [5], except for levels $(^1S^3P)^3P_{0,1,2}$ and $(^1S^3P)^1P_1$. This may be due to strong mixing of terms.

A comparison between the present wavelengths and experimental results obtained from Boiko *et al* [20] is shown in table 4. The difference between each Kα transition was very small. So many Kα transitions were blended in the experiment. The accuracy of the calculated wavelengths (in nm) relative to fitted results can be assessed from table 4, where the agreement is within 0.0124 nm for all available transitions.

The absorption oscillator strengths (f_{ij}) and radiative rate A_{ji} for a transition $i \rightarrow j$ are related by the following expression:

$$f_{ij} = \frac{mc}{8\pi^2 e^2}\lambda_{ji}^2 \frac{\omega_j}{\omega_i} A_{ji} = 1.49 \times 10^{-16} \lambda_{ji}^2 \frac{\omega_j}{\omega_i} A_{ji}, \quad (12)$$

where m and e are electron mass and charge, respectively. c is the velocity of light, λ_{ji} is the transition energy/wavelength in nm, and ω_i and ω_j are the statistical weights of the lower i and upper j levels, respectively. Results for transitions from 1s to 2p are presented. That is to say, transitions for $1s^22s^2$–$1s2s^22p$, $1s^22s2p$–$1s2p^3$, $1s^22s2p$–$1s2s2p^2$ are considered. No data are available for comparing radiative rates and oscillator strengths. So, in this calculation with grasp2K code, the values of radiative rates and oscillator strengths have been determined in both the length and velocity forms, equivalent to the Babushkin and Coulomb gauges in the relativistic nomenclature. It should be noted that transitions with radiative rate ($\geq 10^{-10}$ s) are listed in table 5. The agreement of the two gauges is found to be very good. The nearly equal values of length and velocity forms indicate the accuracy of results. Under the last column in table 5, values of dT have been provided, which is an accuracy indicator and is the deviation of length and velocity form of radiative rates as suggested by Ekman *et al* [21]. The maximum value of dT is 0.0722, which confirms the accuracy of this calculation.

4. Conclusion

In summary, we performed RCI and MCDF method calculations of energy levels of the ground, 5 low-lying and 40 core-excited states in beryllium-like magnesium, Mg IX. Breit interaction and QED were involved in the calculations. The results obtained for wavelength of the Kα transition improve the previous theoretical calculations and compare favourably with the experimental data. The uncertainty of the results was estimated on the basis of an analysis of the convergence of the MCDF results with respect to the length and velocity gauge as suggested by Ekman *et al* [21].

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