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Hyperfine quenching of the $3s3p\ ^3P_0$ level in Mg-like ions

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Abstract

Hyperfine quenching rates of the $3s3p\ ^3P_0$ level in Mg-like ions were calculated using the GRASP2K package based on the multi-configuration Dirac–Hartree–Fock method. Valence and core-valence correlation effects were accounted for in a systematic way. Breit interactions and QED effects were included in the subsequent relativistic CI calculations. Calculated rates were compared with other theoretical values and with experiment, and a good agreement with the latest experimental value for the $^{27}\text{Al}^+$ ion (Rosenband *et al* 2007 *Phys. Rev. Lett.* **98** 220801) was found. Furthermore, we showed in detail the contributions from Breit interaction and QED effects to concerned physical properties. Finally, electronic data were presented in terms of a general scaling law in Z that, given isotopic nuclear spin and magnetic moment, allows hyperfine-induced decay rates to be estimated for any isotope along the isoelectronic sequence.

1. Introduction

In the presence of hyperfine interaction, the atomic state wavefunctions with different electronic angular momentum J are mixed, and then the electronic angular momentum J is not a good quantum number. Therefore, the selection rules on angular momentum apply to the total angular F , which couples the nuclear angular momentum I and the electronic angular J , but not to the electronic angular momentum J . Then some of the transitions forbidden by selection ruled on J may be induced. It is the so-called hyperfine quenching effect, leading to hyperfine-induced transitions (HIT). Since Bowen first predicted this effect (note added in [1]) in 1930, much work has been performed from different theoretical and experimental aspects [2–10]. For example, the HITs of alkaline-earth-like atoms and ions were investigated for realizing ultraprecise atomic clocks, and high-resolution spectroscopy results were

available for Al^+ [11], Zn^+ [12], Sr^+ [13], In^+ [14] and Yb^+ [15]. Also, it is of astrophysical interest to determine isotopic abundance ratios and densities of plasma [16]. Additionally, the HITs may be used to infer nuclear properties [17–20] and probe new physics beyond the standard model such as the weak interaction in atoms [21–23].

Some works on hyperfine quenching of the $3s3p\ ^3P_0$ state of Mg-like ions were available in the literature. The most extensive study was carried out by Marques *et al* [24] using the complex matrix method developed by Indelicato [2]. In these studies, correlations were limited to the outer electrons, which may impair the accuracy for lower Z where core-valence effects are large. Later, rates were also calculated by Brage *et al* using a perturbative approach [16] in order to determine isotopic abundance ratios and diagnose densities of low-density plasmas. Their calculations were restricted to those elements that are abundant in stellar atmospheres. Therefore, accurate theoretical hyperfine-induced $3s3p\ ^3P_0 \rightarrow 3s^2\ ^1S_0$ transition probabilities of Mg-like ions are still scarce.

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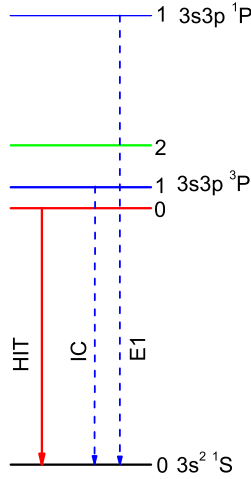


Figure 1. Energy level and transition scheme for Mg-like ions. HIT represents the hyperfine-induced transition, IC the spin-forbidden electrical dipole transition and E1 the resonance electrical dipole transition.

In particular, Rosenband *et al* have recently measured the rates of $^{27}\text{Al}^+$ ions with high precise using quantum logic spectroscopy (QLS) technology [11]. In response to this, we performed further investigations into the hyperfine-induced transition rates of the $3s3p^3P_0$ state for Mg-like ions with $Z = 13 - 78$ using the GRASP2K package [25] based on the multi-configuration Dirac–Hartree–Fock method. The contributions from Breit interaction and QED effects to the HIT rates were also showed. We also gave a scaling law in Z for the hyperfine-induced $3s3p^3P_0 \rightarrow 3s^2 1S_0$ transition in order to estimate the rates for any ion along the Mg-like isoelectronic sequence.

2. Theory

In the presence of the hyperfine interactions, only F and M_F are good quantum numbers, and the wavefunction for a state can be written as

$$|\Gamma F M_F\rangle = \sum_i h_i |\gamma_i J I F M_F\rangle, \quad (1)$$

where $F = I + J$ is the total angular momentum, M_F is the corresponding magnetic quantum number. The zero-order functions $|\gamma J I F M_F\rangle$ in the expansion are coupled products of electronic $|\gamma J M_J\rangle$ and nuclear $|I M_I\rangle$ wavefunctions. The $3s^2 1S_0$ ground state is well represented by a single term. For $3s3p^3P_0$ only the interaction with $3s3p^{1,3}P_1$ is important (see figure 1), and other states in the expansion can be neglected due to large energy separations and comparatively weak hyperfine couplings. The wavefunction for $3s3p^3P_0$ can thus to a good approximation be represented by the expansion

$$|{}^3s3p^3P_0 I F'\rangle = h_0 |3s3p^3P_0 I F\rangle + \sum_{S=0,1} h_S |3s3p^{(2S+1)}P_1 I F\rangle. \quad (2)$$

The use of quotation marks in the left-hand wavefunction emphasizes the fact that the notation is just a label indicating the dominant character of the eigenvector. The mixing

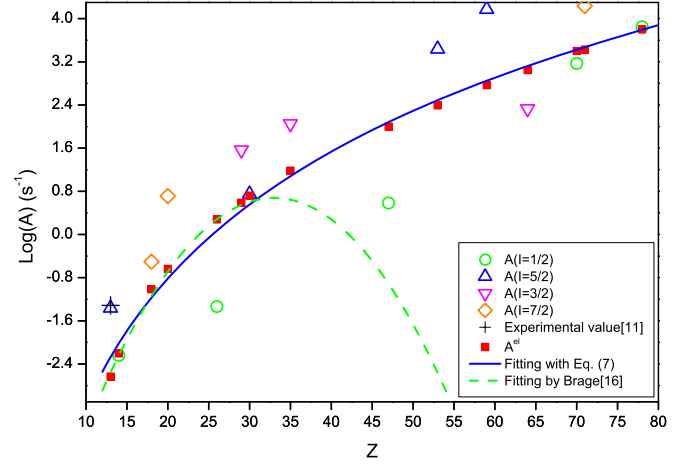


Figure 2. Logarithm of hyperfine-induced rates A with different nuclear spin for $3s3p^3P_0 \rightarrow 3s^2 1S_0$ transition of Mg-like ions together with the experimental value from [11]. Reduced hyperfine-induced decay rates A_{el} and fitted curves are also displayed.

coefficients h_S are obtained in first-order perturbation theory as ratios between hyperfine matrix elements and the unperturbed energy differences

$$h_S = \frac{\langle 3s3p^{(2S+1)}P_1 I F | H_{\text{hfs}} | 3s3p^3P_0 I F \rangle}{E(^3P_0) - E(^{(2S+1)}P_1)}. \quad (3)$$

As can be seen from the above formula, the one photon $3s3p^3P_0 \rightarrow 3s^2 1S_0$ E1 transition becomes allowed via the mixing of $3s3p^{1,3}P_1$. The contribution from the hyperfine quadrupole interaction was neglected since it is fairly small compared with the magnetic dipole interaction. So the corresponding transition probability can be written as [26]

$$A = \frac{2.02613 \times 10^{18}}{3\lambda^3} \left| \sum_{S=0,1} h_S \langle 3s^2 1S_0 || Q_1 || 3s3p^{(2S+1)}P_1 \rangle \right|^2, \quad (4)$$

where Q_1 is the electric dipole tensor operator, A is the decay rate in s^{-1} and λ is the wavelength in \AA for the $3s3p^3P_0 \rightarrow 3s^2 1S_0$ transition. The reduced matrix elements $\langle 3s^2 1S_0 || Q_1 || 3s3p^3P_1 \rangle$ and $\langle 3s^2 1S_0 || Q_1 || 3s3p^1P_1 \rangle$ are square roots of the line strengths. It can be found from equation (4) that there exists an interference effect in the hyperfine quenching of $3s3p^3P_0$ as discussed in [16, 6, 27].

The electronic wavefunctions were computed using the GRASP2K program package [25]. Here, the wavefunction for a state labelled γJ is approximated by an expansion over jj -coupled configuration state functions (CSFs):

$$\Psi(\gamma J) = \sum_j d_j \Phi_j. \quad (5)$$

The configuration state functions are anti-symmetrized linear combinations of products of Dirac orbitals. In the multi-configuration self-consistent field (SCF) procedure both the radial parts of the orbitals and the expansion coefficients are optimized to self-consistency. In the present work a Dirac–Coulomb Hamiltonian was used with the nucleus described

Table 1. Comparison between theoretical and experimental transition energies taken from the NIST Database [37] (in cm^{-1}) and line strengths (in au) of the $3s3p\ ^3P_1-3s^2\ ^1S_0$ and $3s3p\ ^1P_1-3s^2\ ^1S_0$ transitions for selected Mg-like ions. Numbers in brackets represent powers of ten.

Z	Work	$3s3p\ ^3P_1-3s^2\ ^1S_0$			$3s3p\ ^1P_1-3s^2\ ^1S_0$		
		ΔE	S_L	S_V	ΔE	S_L	S_V
13	This work	37 625	8.897[−5]	8.493[−5]	60 065	9.732	9.390
	MCDF(1996) [35]	36 689	7.492[−5]		60 696	9.620	
	MCDF(1997) [34]	37 253	8.037[−5]	7.712[−5]	60 104	9.609	9.680
	MCDHF(2001) [32]	37 543	8.754[−5]	9.200[−5]	60 224	9.678	9.801
	Exp.	37 454	9.376[−5] ^a 9.236[−5] ^c		59 852	9.572 ^b	
14	This work	52 859	1.667[−4]	1.749[−4]	82 898	6.602	6.463
	MCDF(1996) [35]	51 945	1.460[−4]		84 207	6.346	
	MCDF(1997) [34]	52 606	1.591[−4]	1.633[−4]	83 104	6.395	6.435
	CIV3(2000) [33]				83 254	6.710	
	MCDHF(2001) [32]	52 886	1.670[−4]	1.732[−4]	83 185	6.418	6.493
	Exp.	52 853	1.675[−4] ^d		82 884		
18	This work	113 757	8.071[−4]	8.397[−4]	170 765	2.282	2.373
	MCDF(1996) [35]	112 698	7.821[−4]		173 822	2.258	
	MCDF(1997) [34]				170 977	2.269	2.284
	CI(1999) [36]				171 068	2.297	
	MCDHF(2001) [32]	113 770	8.050[−4]		170 864	2.272	
	Exp.	113 904			170 722	2.254 ^e	
26	This work	239 303	4.588[−3]	4.718[−3]	351 713	7.310[−1]	7.342[−1]
	MCDF(1996) [35]	237 949	4.399[−3]		355 768	7.325[−1]	
	CIV3(2000) [33]				362 199	7.331[−1]	
	MCDHF(2001) [32]	239 528	4.647[−3]		352 143	7.338[−1]	
	Exp.	239 660			351 911		
35	This work	394 620	1.309[−2]	1.320[−2]	598 765	3.261[−1]	3.267[−1]
	MCDHF(2001) [32]	394 077	1.321[−2]		599 857	3.283[−1]	
	Exp.	394 255	1.300[−2] ^f				
47	This work	621 972	2.072[−2]	2.153[−2]	1111 335	1.467[−1]	1.483[−1]
	MCDHF(2001) [32]	623 735	2.089[−2]		1112 652	1.479[−1]	
70	This work	1141 070	1.510[−2]	1.649[−2]	3597 981	5.143[−2]	5.277[−2]
	MCDHF(2001) [32]	1144 516	1.525[−2]		3599 130	5.173[−2]	

^a Johnson *et al* [38].^b Kernaha *et al* [39].^c Trabert *et al* [40].^d Kwong *et al* [41].^e Reistad *et al* [42].^f Träbert *et al* [43].

by an extended Fermi charge distribution [28]. The multi-configuration SCF calculations were followed by relativistic CI calculations (RCI) including the Breit interaction and leading QED effects.

3. Results and discussion

3.1. Computational model and method

An important factor influencing the accuracy of the HIT probability is the electronic correlation effect, especially for low charged ions. As a starting point SCF calculations were performed for, respectively, the $3s^2$ and $3s3p$ configurations in the extended optimal level (EOL) mode with the $(2J + 1)$ weighted energy average of all the fine-structure levels. These calculations were followed by calculations with expansions obtained by single and double replacements from the reference configuration $3s^2$ of the ground state and $3s3p$ of the excited

state to active sets up to $n \leq 6, \ell = 5$. For $Z \leq 20$, orbitals with $n \leq 7, \ell = 5$ were also included. Due to stability problems in the relativistic SCF procedure, only the outermost layers of orbitals could be optimized each time for the large active set. The core polarization from 2s and 2p shells was taken into account in the following relativistic configuration interaction (RCI) calculations by diagonalizing the Coulomb Hamiltonian matrix. Furthermore, Breit interaction and vacuum polarization can be included into the Hamiltonian [29], and the approximate self-energy correction was evaluated using a screened hydrogenic model [29]. An obvious difference from previous GRASP92 package [30] is that self-energy correction can be accumulated in this matrix [31]. Then through diagonalizing the corresponding Hamiltonian matrix, the configuration mixing coefficients d_j in equation (5) were further optimized, and a more accurate atomic state wavefunction was obtained.

Table 2. Transition energies (in cm^{-1}) and line strengths (in au) for the $3s3p\ ^3P_1-3s^2\ ^1S_0$ and $3s3p\ ^1P_1-3s^2\ ^1S_0$ transitions. Breit interaction and QED corrections have been included. Numbers in brackets represent powers of ten.

Z	S($3s3p\ ^3P_1-3s^2\ ^1S_0$)		S($3s3p\ ^1P_1-3s^2\ ^1S_0$)	
	ΔE	S_L	ΔE	S_L
13	37 625	8.897[-5]	60 065	9.732
14	52 859	1.667[-4]	82 898	6.602
18	113 757	8.071[-4]	170 765	2.282
20	143 499	1.374[-3]	214 662	1.601
26	239 303	4.588[-3]	351 713	7.310[-1]
29	287 960	7.111[-3]	426 595	5.413[-1]
30	306 395	8.027[-3]	452 970	4.937[-1]
35	394 620	1.309[-2]	598 765	3.261[-1]
47	621 972	2.072[-2]	1111 335	1.467[-1]
53	746 367	2.063[-2]	1509 550	1.061[-1]
59	877 028	1.908[-2]	2052 697	7.990[-2]
64	992 792	1.732[-2]	2651 103	6.469[-2]
70	1141 070	1.510[-2]	3597 981	5.143[-2]
71	1168 285	1.474[-2]	3784 167	4.958[-2]
78	1357 748	1.236[-2]	5371 293	3.901[-2]

Table 3. Comparison of present hyperfine matrix elements with those of Marques *et al* in eV. $W_{3,0}$ represents $\langle 3s3p\ ^3P_1 IF | H_{\text{hfs}} | 3s3p\ ^3P_0 IF \rangle$, $W_{1,0}$ represents $\langle 3s3p\ ^1P_1 IF | H_{\text{hfs}} | 3s3p\ ^3P_0 IF \rangle$. Magnetic dipole moments (in μ_N) are taken from the tabulation by Stone [44]. Numbers in brackets represent powers of ten.

Z	I	μ_I	$W_{3,0}$		$W_{1,0}$	
			This work	[24]	This work	[24]
13	5/2	3.641 5069	1.615[-5]		1.290[-5]	
14	1/2	0.555 29	5.646[-6]	5.031[-6]	4.353[-6]	3.914[-6]
18	7/2	1.588	4.026[-5]		3.016[-5]	
20	7/2	1.317 3	5.392[-5]	5.085[-5]	3.986[-5]	3.804[-5]
26	1/2	0.090 44	1.745[-5]	1.654[-5]	1.151[-5]	1.121[-5]
29	3/2	2.381 6	5.266[-4]	5.109[-4]	3.275[-4]	3.209[-4]
30	5/2	0.875 2049	2.097[-4]	1.979[-4]	1.230[-4]	1.207[-4]
35	3/2	2.106 4	1.026[-3]	9.795[-4]	5.096[-4]	5.030[-4]
47	1/2	0.113 57	2.270[-4]	2.360[-4]	7.109[-5]	7.296[-5]
53	5/2	2.813 27	6.401[-3]	6.530[-3]	1.563[-3]	1.567[-3]
59	5/2	4.275 4	1.566[-2]	1.553[-2]	2.931[-3]	2.945[-3]
64	3/2	0.339 8	1.924[-3]	1.895[-3]	3.005[-4]	3.001[-4]
70	5/2	0.648 0	5.014[-3]	5.227[-3]	6.393[-4]	6.770[-4]
71	7/2	2.232 3	1.767[-2]	1.760[-2]	2.184[-3]	2.208[-3]
78	1/2	0.609 52	1.153[-2]	1.146[-2]	1.147[-3]	1.159[-3]

In order to infer the accuracy of our computational method, the transition energies and the line strengths for the $3s3p\ ^3P_1-3s^2\ ^1S_0$ electrical dipole transitions were compared with other theoretical and experimental values [32–43] in table 1. The present transition energies are in good agreement with experimental and other theoretical values. For the resonance transition of $3s^2\ ^1S_0 \rightarrow 3s3p\ ^1P_1$, the line strengths from the Babushkin gauge and Coulomb gauge agree to about 3%. For the intercombination line $3s^2\ ^1S_0 \rightarrow 3s3p\ ^3P_1$ there is an agreement to about 5%. The values are consistent with other theoretical calculations except for these results obtained by Stanek *et al* [35] using the MCDHF method. The reason is due to limited correlation in their calculation. In the following calculations, the line strength in the Babushkin gauge would be used. All transition energies and line strengths in the Babushkin (length) gauge for Mg-like ions between $Z = 13 - 78$ are given in table 2.

Calculated off-diagonal hyperfine matrix elements $\langle 3s3p\ ^{2S+1}P_1 IF | H_{\text{hfs}} | 3s3p\ ^3P_0 IF \rangle$, labelled $W_{2S+1,0}$, are

listed in table 3. Nuclear parameters used in these computations were taken from [44]. As can be seen from this table, the current values for low Z ions differ substantially from those by Marques *et al* [24]. The difference may be attributed to limited correlation in the pioneering calculation by Marques. Inconsistent nuclear data also add to the difference. As the atomic number Z increases, electron correlation effects decrease and the agreement is better.

3.2. Hyperfine-induced transition probability

Given expansion coefficients h_S and the relevant line strength, the hyperfine-induced $3s3p\ ^3P_0 \rightarrow 3s^2\ ^1S_0$ transition probability can be obtained by equation (4). Present calculational results are given in table 4 together with the corresponding wavelengths and other theoretical and experimental values. In this table, PT denotes perturbative results by Brage *et al* [16], CM are complex matrix results obtained by Marques *et al* [24]. As can be seen from this

Table 4. Wavelengths (λ), probabilities (A) and reduced rates (A_{el}) for hyperfine induced transition $3s^2\ ^1S_0-3s3p\ ^3P_0$ in Mg-like ions. Magnetic dipole moments (in μ_N) are taken from [44]. The results are compared with other theoretical and experimental values. PT and CM refer to perturbative and complex matrix results, respectively. Numbers in brackets represent powers of ten.

Z	I	μ_1	$\lambda(\text{\AA})$		A_{el}	A (s^{-1})				
			This work	Exp. [37]		This work	CM [24]	PT [16]	Exp. [11]	
13	5/2	3.641 5069	2669.080	2679.811	2.331[-3]	4.327[-2]				4.854[-2]
14	1/2	0.555 29	1901.352	1900.529	6.227[-3]	5.760[-3]	3.545[-3]	5.23[-3]		
18	7/2	1.588	887.575	886.476	9.641[-2]	3.126[-1]				
20	7/2	1.317 3	706.070	699.862	2.306[-1]	5.144[-1]	3.851[-1]	4.79[-1]		
26	1/2	0.090 44	429.275	428.509	1.895	4.649[-2]	3.858[-2]	4.98[-2]		
29	3/2	2.381 6	360.191	358.105	3.889	3.676[1]	2.930[1]			
30	5/2	0.875 2049	339.548	339.390	5.249	5.629	4.275			
35	3/2	2.106 4	267.978	268.230	1.525[1]	1.128[2]	9.320[1]			
47	1/2	0.113 57	175.634		9.97[1]	3.858	4.735[1]			
53	5/2	2.813 27	147.767		2.466[2]	2.732[3]	3.489[3]			
59	5/2	4.275 4	126.523		5.833[2]	1.493[4]	1.898[4]			
64	3/2	0.339 8	112.102		1.110[3]	2.136[2]	2.753[2]			
70	5/2	0.648	97.398		2.514[3]	1.478[3]	2.036[3]			
71	7/2	2.232 3	95.429		2.678[3]	1.715[4]	2.296[4]			
78	1/2	0.609 52	82.121		6.318[3]	7.042[3]	9.506[3]			

Table 5. The contributions of Coulomb, Breit interaction, vacuum polarization and self-energy to the total hyperfine matrix elements $W_{3,0}$ and $W_{1,0}$ (in au), the transition energies (in cm^{-1}) and line strengths (in au) for the $3s3p\ ^3P_1-3s^2\ ^1S_0$ and $3s3p\ ^1P_1-3s^2\ ^1S_0$ transitions for Mg-like Al, Fe, Ag, Yb, respectively. CI represents the contribution from Coulomb interaction, BI Breit interaction, VP vacuum polarization and SE self-energy correction. Numbers in brackets represent powers of ten.

Ions	Models	W_{30}	W_{10}	$3s3p\ ^3P_1-3s^2\ ^1S_0$		$3s3p\ ^1P_1-3s^2\ ^1S_0$	
				ΔE	S_L	ΔE	S_L
Al ⁺	CI	1.614[-5]	1.289[-5]	37 615	8.834[-5]	60 089	9.682
	BI	0.005[-5]	0.001[-5]	4	-0.018[-5]	40	0.001
	VP	0	0	0	0	32	0
	SE	-0.004[-5]	0	6	0.081[-5]	-96	0.049
	Total	1.615[-5]	1.290[-5]	37 625	8.897[-5]	60 065	9.732
Fe ¹⁴⁺	CI	1.735[-5]	1.149[-5]	239 779	4.812[-3]	352 107	7.304[-1]
	BI	0.004[-5]	0.002[-5]	369	-0.225[-3]	60	0.007[-1]
	VP	0.009[-5]	0	50	0	57	0
	SE	-0.003[-5]	0	-895	0.001[-3]	-511	-0.001[-1]
	Total	1.745[-5]	1.151[-5]	239 303	4.588[-3]	351 713	7.310[-1]
Ag ³⁵⁺	CI	2.269[-4]	7.267[-5]	623 835	2.091[-2]	1117 536	1.465[-1]
	BI	0	0.038[-5]	5131	-0.023[-2]	396	0.004[-1]
	VP	0.001[-4]	0.003[-5]	894	0.006[-2]	930	0
	SE	0	-0.199[-5]	-7888	-0.002[-2]	-7527	-0.002[-1]
	Total	2.270[-4]	7.109[-5]	621 972	2.072[-2]	1111 335	1.467[-1]
Yb ⁵⁸⁺	CI	5.090[-3]	6.397[-4]	115 002 2	1.547[-2]	3626 456	5.161[-2]
	BI	-0.084[-3]	0.008[-4]	24 456	-0.030[-2]	486	0.011[-2]
	VP	0.007[-3]	0.144[-4]	6032	0.010[-2]	6614	0.001[-2]
	SE	0.001[-3]	-0.156[-4]	-39440	-0.017[-2]	-35575	-0.040[-2]
	Total	5.014[-3]	6.393[-4]	114 107 0	1.510[-2]	3597 981	5.143[-2]

table, the agreement between our results and the values of Brage *et al* is acceptable. Whereas the CM values differ from the present results and those of Brage *et al* mainly for two reasons: limited correlation included in the Marques *et al* calculation, which can be seen in the off-diagonal hyperfine matrix elements listed in table 3, and the inherent problems with the transition energies used in the CM method [27].

We further compared present calculations with the latest experimental measurements [11], a good agreement for the hyperfine-induced rate of ²⁷Al⁺ was found.

In tables 5 and 6, we further show some details of the contributions from Coulomb interaction (CI), Breit interaction (BI) and QED effects including vacuum polarization (VP) and self-energy (SE) to different physical quantities for Mg-like Al,

Table 6. The contributions of Coulomb, Breit interaction, vacuum polarization and self-energy to the wavelength (in Å), hyperfine mixing coefficient h_S (in au), reduced hyperfine induced transition probability A_{el} (in s^{-1}) and hyperfine induced transition probability A (in s^{-1}) for Mg-like Al, Fe, Ag, Yb. CI represents the contribution from Coulomb interaction, BI Breit interaction, VP vacuum polarization and SE self-energy correction. Numbers in brackets represent powers of ten.

Ions	Models	$\lambda(\text{Å})$	h_1	h_0	A_{el}	A
Al ⁺	CI	2668.254	2.134[−3]	4.614[−6]	2.264[−3]	4.203[−2]
	BI	−0.329	0.041[−3]	−0.005[−6]	0.047[−3]	0.087[−2]
	VP	−0.139	0.039[−3]	−0.006[−6]	0	0.001[−2]
	SE	1.294	−0.041[−3]	0.021[−6]	0.020[−3]	0.037[−2]
	Total	2669.080	2.173[−3]	4.624[−6]	2.331[−3]	4.327[−2]
Fe ¹⁴⁺	CI	428.929	2.323[−5]	7.830[−7]	1.814	4.450[−2]
	BI	−0.901	0.084[−5]	0.047[−7]	0.051	0.125[−2]
	VP	−0.199	0.049[−5]	0.005[−7]	0.058	0.144[−2]
	SE	1.446	−0.003[−5]	−0.025[−7]	−0.028	−0.071[−2]
	Total	429.275	2.453[−5]	7.857[−7]	1.895	4.649[−2]
Ag ³⁵⁺	CI	175.313	3.525[−5]	1.074[−6]	9.825[1]	3.802
	BI	−1.813	0.064[−5]	0.017[−6]	5.752	0.222
	VP	−0.266	−0.011[−5]	0.001[−6]	0.102	0.006
	SE	2.400	0.005[−5]	−0.030[−6]	−4.390	−0.172
	Total	175.634	3.583[−5]	1.062[−6]	9.972[1]	3.858
Yb ⁵⁸⁺	CI	97.104	3.509[−4]	1.989[−6]	2.439[3]	1.434[3]
	BI	−2.479	0.006[−4]	0.023[−6]	0.156[3]	0.092[3]
	VP	−0.533	−0.003[−4]	0.045[−6]	0.059[3]	0.034[3]
	SE	3.306	0.110[−4]	−0.050[−6]	−0.140[3]	−0.082[3]
	Total	97.398	3.622[−4]	2.007[−6]	2.514[3]	1.478[3]

Fe, Ag and Yb. As can be seen from these two tables, both Breit interaction and QED effect together correct the hyperfine mixing coefficient h_1 , h_0 and the HIT rates by less than 5.5%, 1.5% and 5%, respectively.

In order to establish systematic trends for hyperfine quenching rates along the isoelectronic sequence, we factorized the hyperfine-induced transition rate into nuclear and electronic parts (see Brage *et al* [16]),

$$A(^3P_0 \rightarrow ^1S_0) = [\mu_I^2(1 + I^{-1})]A_{el}(^3P_0 \rightarrow ^1S_0). \quad (6)$$

The reduced hyperfine-induced transition rates A_{el} are relatively independent of nuclear effects. In figure 2, the reduced and total hyperfine-induced transition rates are shown along the isoelectronic sequence. The electronic part A_{el} has a smooth behaviour along the isoelectronic sequence.

To estimate the transition rate for any isotope, we fit a power function in Z :

$$A_{el} = 1.087 \times 10^{-11} Z^{7.8004}. \quad (7)$$

The fitted function is shown in figure 2 and it gives a global description of the data. Higher accuracy can be obtained by spline interpolation based on the A_{el} values in table 4. In the figure, the polynomial fit by Brage *et al*, which is valid only for low Z , is also displayed.

4. Conclusion

In summary, hyperfine-induced $3s3p^3P_0 \rightarrow 3s^2^1S_0$ transition probabilities of Mg-like ions with $Z = 13 - 78$ were

calculated using GRASP2K based on the multi-configuration Dirac–Hartree–Fock method. Accurate theoretical transition rates were obtained for the full sequence, especially a good agreement with the recent experimental value for $^{27}\text{Al}^+$ [11] was found. The detailed list of the contributions of the Breit interaction and QED effect to relevant physical magnitudes was shown. A fitting formula in Z for the reduced transition rates was further derived in order to predict the hyperfine-induced $3s3p^3P_0 \rightarrow 3s^2^1S_0$ transition rate for any isotope of Mg-like ions.

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