Hyperfine induced $1s2s \, ^1S_0 \rightarrow 1s^2 \, ^1S_0$ M1 transition of He-like ions

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Abstract

Hyperfine induced $1s2s \, ^1S_0 \rightarrow 1s^2 \, ^1S_0$ M1 transition probabilities of He-like ions have been calculated from relativistic configuration interaction wavefunctions including the frequency independent Breit interaction and QED effects. Present results for $^{151}$Eu and $^{155}$Gd are in good agreement with previous calculations [Phys. Rev. A 63, 054105 (2001)]. Electronic data are given 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. The results should be helpful for future experimental investigations on QED and parity non-conservation effects.

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The hyperfine structure of atomic levels is caused by the interaction between the electrons and the non-central electromagnetic multipoles of the nucleus. The interaction, although weak, not only shifts and splits the individual $J$ levels, but also mixes wavefunctions with different $J$ quantum numbers [1]. The mixing may open new decay channels and induce radiative transitions such as $J = 0 \rightarrow J' = 0$. The study of hyperfine induced transitions (HIT) is attractive in view of getting a more subtle understanding of electron correlation and relativistic effects [2, 3, 4], testing the standard model [5], obtaining nuclear properties [6, 7, 8], developing ultra-precise atomic clocks [9, 10, 11, 12], analyzing stellar spectra [13], and determining isotopic abundance ratios and electron densities of plasma [14, 15].

He-like systems are interesting due to their relative simplicity, and important effects such as electron correlation [10], quantum electrodynamics (QED) [17, 18, 19] and parity non-conservation (PNC) phenomena [20, 21, 22, 23] can be investigated in detail. Gorshkov and Labzovskii [20] and Labzowsky et al. [23] have proposed that the mixed hyperfine- and weak-quenching can be used to test parity-violation effects. The one photon transition $1s2s \, ^1S_0 \rightarrow 1s^2 \, ^1S_0$ of He-like ions is considered a good candidate for these tests and experiments will be carried out at GSI [24]. Therefore, accurate hyperfine induced $1s2s \, ^1S_0 \rightarrow 1s^2 \, ^1S_0$ M1 transition probabilities of He-like ions are important. Relevant data are however still insufficient and in response to this we have performed systematic calculations along the He-like iso-electronic sequence using GRASP2K [25] based on the multi-configuration Dirac-Hartree-Fock method and the HFST [26] package. From computed hyperfine induced transitions for 14 ions and corresponding electronic quantities we have derived a scaling formula in $Z$ that allows the induced transition rate to be computed for any isotope.

When the hyperfine interaction is included the wavefunctions of the combined electronic and nuclear system can be represented as

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

The zero-order functions $|\gamma J I F M_F \rangle$ in the expansion are coupled products of electronic $|\gamma J M_f \rangle$ and nuclear $|I M_I \rangle$ wavefunctions. The $1s^2 \, ^1S_0$ ground state is well represented by a single term. For $1s2s \, ^1S_0$ only the interaction with $1s2s \, ^3S_1$ is important (see Figure 1) and the wavefunction can be approximated by the expansion

$$|\langle 1s2s \, ^1S_0 IF \rangle \rangle = c_0 |1s2s \, ^1S_0 IF \rangle + c_1 |1s2s \, ^3S_1 IF \rangle, \quad (2)$$

where $I$ is the nuclear spin and $F (= I)$ the total angular momentum quantum number. Magnetic quantum numbers are suppressed for brevity. 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 coefficient $c_1$ is obtained in first order perturbation theory as the ratio between the hyperfine matrix element and the unperturbed energy differences

$$c_1 = \frac{\langle 1s2s \, ^3S_1 IF |H_{hf,x}|1s2s \, ^1S_0 IF \rangle}{E(1S_0) - E(^3S_1)}. \quad (3)$$

The one-photon $1s2s \, ^1S_0 \rightarrow 1s^2 \, ^1S_0$ M1 transition becomes allowed via the mixing of $1s2s \, ^3S_1$ and the decay rate in s$^{-1}$ is given by

$$A_{HIT}(1s2s \, ^1S_0 \rightarrow 1s^2 \, ^1S_0) = \frac{2.69735 \times 10^{13} c_1^2 S_{M1}}{3\lambda^3}, \quad (4)$$

where

$$S_{M1} = |\langle 1s^2 \, ^1S_0 |M^{(1)}|1s2s \, ^3S_1 \rangle|^2 \quad (5)$$

is the line strength computed from unperturbed wavefunctions. $\lambda$ is the wavelength in Å for the transition. The reader is referred to [14, 27, 28] for details of the derivation.
The electronic wavefunctions were computed using the GRASP2K program package [24]. Here the wavefunction for a state labeled $\gamma J$ is approximated by an expansion over $jj$-coupled configuration state functions (CSFs)

$$|\gamma J\rangle = \sum_i d_i \Phi_i.$$  

(6)

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 by an extended Fermi charge distribution [29]. The multi-configuration SCF calculations were followed by relativistic CI calculations including the frequency independent Breit interaction and leading QED effects.

For the low charged ions the main uncertainties in the calculation come from electron correlation effects. To build a reasonable correlation model and control the accuracy we performed tentative calculations of transition energies and the $\langle 1s2s\,3S_1 \mid IF \mid H_{bf} \mid 1s2s\,1S_0 \,IF \rangle$ off-diagonal hyperfine matrix element in $^{12}\text{C}$. In the calculations the wavefunctions for $1s^2\,1S_0$, $1s2s\,1S_0$, $1s2s\,3S_1$ were determined simultaneously in extended optimal level (EOL) calculations [30]. All CSFs that could be built from an active set of orbitals were included in the expansion. The orbital set was systematically increased by adding layers of new orbitals. The largest active set included relativistic orbitals with principal quantum number $n \leq 7$. Due to stability problems in the relativistic SCF procedure only the outermost layers of orbitals could be optimized each time. The frequency independent Breit interaction and leading QED effects were added in subsequent relativistic CI calculations. The results for $^{12}\text{C}$ are shown in Table 1. The first column in this table represent the active set of orbitals involved in each step of the calculation. As can be seen from the table, five energy-optimized layers of orbitals are needed to converge the off-diagonal hyperfine interaction matrix element between $1s2s\,3S_1$ and $1s2s\,1S_0$ at a sub per mill level.

Based on the above analysis, we performed calculations for other He-like ions using an active orbital set with $n \leq 5$. The Breit interaction and main QED corrections were included. Values of nuclear magnetic dipole moments for the different isotopes were adopted from the compilation by Stone [32]. In Table 2 we display the off-diagonal hyperfine matrix elements and corresponding mixing coefficients $c_1$. The given values are not corrected for the the anomalous magnetic moment. For the mixing coefficient of $^{151}\text{Eu}$ the magnitude is agreement with the value of [23], but with a difference in sign due to different definitions of the phase factor in the hyperfine interaction matrix element. The difference in sign does not influence the final hyperfine induced transition probability. Wavelengths $\lambda$ and line strengths $S_{M1}$ for the $1s2s\,3S_1 \rightarrow 1s^2\,1S_0$ M1 transition needed for the quenching rate are taken from accurate relativistic CI calculations by Johnson et al. [18]. The values are presented in Table 3 for the convenience of the reader. The hyperfine induced $1s2s^3S_0 \rightarrow 1s^2\,1S_0$ M1 transition rate and corresponding wavelengths of He-like ions are given Table 4. Previous theoretical results of wavelength [33] are compared with present calculations in this table. The agreement between our value for $^{151}\text{Eu}$ and previous theoretical values by Labzowsky et al. [23] is very good.

To predict the transition rate for any isotope in the iso-electronic sequence we follow Brage et al. [14] and factorize the hyperfine induced transition rate into nuclear and electronic parts

$$A_{HIT}(1s2s\,1S_0 \rightarrow 1s^2\,1S_0) = \mu^2(1 + 1/I)A^{el}(1s2s\,1S_0 \rightarrow 1s^2\,1S_0).$$  

(7)

The electronic part $A^{el}$ has a smooth behavior along the iso-electronic sequence making interpolation possible. From the data in Table 4 we obtain a fit of the form

$$A^{el} = 1.9728 \times 10^{-19} Z^{14.065}$$  

(8)

where $Z$ is the atomic number. The fit is shown in Figure 2. In order to show clearly the trend of $A^{el}$ with $Z$, log(A) was plotted in this picture. Using the fitting formula we estimate the probability of $^{155}\text{Gd}$ with nuclear spin $I = 3/2$ and nuclear dipole moment $\mu = -0.2591\mu_N$ to be $5.60 \times 10^5$ s$^{-1}$. This value is in good agreement with the theoretical value $5.8 \times 10^5$ s$^{-1}$ given in [23]. The fitting formula (8) is expected to provide accurate values, but further examination through experiment and theory is still needed.
To sum up we have calculated hyperfine induced $1s^2 1S_0 \rightarrow 1s^2 1S_0$ M1 transition probabilities of He-like ions using GRASP2K [25] based on multi-configuration Dirac-Fock method and the HFST [26] package. Electron correlation effects were included in a systematic way. The Breit interaction and QED effects were included in subsequent relativistic CI calculations. A scaling law in $Z$ was derived for the electronic quantities. The scaling law allows hyperfine induced transition probabilities to be estimated for any isotope.

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Figure 1: Level structure of the 1s^2, 1s2s and 1s3s configurations in He-like C and Ir.

Table 1: Transition energies in cm\(^{-1}\) and off-diagonal hyperfine interaction matrix element in a.u. for \(^{12}\text{C}\) from calculations with increasing active sets. \(\Delta E_1 = E(1s2s \ ^3S_1) - E(1s^2 \ ^1S_0)\), \(\Delta E_2 = E(1s2s \ ^1S_0) - E(1s2s \ ^1S_1)\), \(\Delta E_3 = E(1s2s \ ^3S_1) - E(1s2s \ ^3S_1)\).

| active set | \(\Delta E_1\) | \(\Delta E_2\) | \(\Delta E_3\) | Matrix Element |
|------------|---------------|---------------|---------------|----------------|
| 2s1p       | 2407416       | 2451264       | 43847         | 4.3613[-6]     |
| 3s2p1d     | 2410850       | 2455165       | 44315         | 4.5773[-6]     |
| 4s3p2d1f   | 2411282       | 2455181       | 43899         | 4.5641[-6]     |
| 5s4p3d1g   | 2411308       | 2455148       | 43840         | 4.5576[-6]     |
| 6s5p4d3g1h | 2411422       | 2455224       | 43802         | 4.5576[-6]     |
| 7s6p5d4g2h1i | 2411475 | 2455265       | 43791         | 4.5575[-6]     |
| QED corrections | 2411439 | 2455237       | 43798         | 4.5572[-6]     |
| Experiment [31] | 2411271   | 2455026       | 43755         |                 |

Table 2: Off-diagonal hyperfine interaction matrix elements (a.u.) and hyperfine mixing coefficients \(c_1\) of He-like ions. Nuclear magnetic dipole moment \(\mu_I\) are from [32].

| Isotope | Z | I   | \(\mu_I\) | Matrix Element | Mixing Coefficient |
|---------|---|-----|----------|----------------|-------------------|
| \(^{12}\text{C}\) | 6 | 1/2 | 0.7042   | 4.5576[-6]     | 2.2817[-5]        |
| \(^{19}\text{F}\) | 9 | 1/2 | 2.62868  | 5.7260[-5]     | 1.6993[-4]        |
| \(^{28}\text{Si}\) | 14 | 1/2 | -0.55529 | -4.5667[-5]    | -8.1505[-5]       |
| \(^{47}\text{Ti}\) | 22 | 5/2 | -0.78848 | -1.7489[-4]    | -1.8463[-4]       |
| \(^{57}\text{Fe}\) | 26 | 1/2 | 2.56277  | 4.8981[-5]     | 4.2385[-5]        |
| \(^{70}\text{Ga}\) | 31 | 3/2 | 2.6289   | 1.7944[-3]     | 1.2473[-3]        |
| \(^{85}\text{Rb}\) | 37 | 5/2 | 1.35298  | 1.5213[-3]     | 8.4420[-4]        |
| \(^{97}\text{Mo}\) | 42 | 5/2 | -0.9335  | -1.5826[-3]    | -7.3716[-4]       |
| \(^{103}\text{Rh}\) | 45 | 1/2 | -0.884   | -2.7542[-3]    | -1.1627[-3]       |
| \(^{117}\text{Sn}\) | 50 | 1/2 | -1.00104 | -4.4439[-3]    | -1.6030[-3]       |
| \(^{131}\text{Xe}\) | 54 | 3/2 | 0.6908   | 2.9782[-3]     | 9.5300[-4]        |
| \(^{151}\text{Eu}\) | 63 | 5/2 | 3.4717   | 2.3846[-2]     | 5.8619[-3]        |
| \(^{175}\text{Lu}\) | 71 | 7/2 | 2.2323   | 2.3187[-2]     | 4.5372[-3]        |
| \(^{193}\text{Ir}\) | 77 | 3/2 | 0.1637   | 2.6895[-3]     | 4.4400[-4]        |
Table 3: Wavelengths $\lambda$ in Å, rates $A_{M1}$ in s$^{-1}$ and line strengths $S_{M1}$ in a.u. for the $1s2s^3S_1 - 1s^21S_0$ M1 transition of He-like ions. From Johnson et al. [18].

| Ion  | Z  | $\lambda$ (Å) | $A_{M1}$ | $S_{M1}$ |
|------|----|----------------|----------|----------|
| C    | 6  | 41.470         | 4.860[1] | 3.8550[-7] |
| F    | 9  | 17.152         | 3.621[3] | 2.0323[-6] |
| Si   | 14 | 6.7402         | 3.598[5] | 1.2253[-5] |
| Ti   | 22 | 2.6368         | 3.750[7] | 7.6467[-5] |
| Fe   | 26 | 1.8682         | 2.075[8] | 1.5046[-4] |
| Ga   | 31 | 1.3002         | 1.257[9] | 3.0719[-4] |
| Rb   | 37 | 0.90272        | 7.714[9] | 6.3110[-4] |
| Mo   | 42 | 0.69459        | 2.842[10]| 1.0592[-3] |
| Rh   | 45 | 0.60198        | 5.792[10]| 1.4054[-3] |
| Sn   | 50 | 0.48342        | 1.726[11]| 2.1681[-3] |
| Xe   | 54 | 0.41151        | 3.846[11]| 2.9807[-3] |
| Eu   | 63 | 0.29715        | 1.943[12]| 5.6695[-3] |
| Lu   | 71 | 0.22993        | 6.950[12]| 9.3969[-3] |
| Ir   | 77 | 0.19266        | 1.672[13]| 1.3300[-2] |

Table 4: Hyperfine induced rates $A_{HIT}$ in s$^{-1}$ and corresponding wavelength $\lambda$ in Å for the $1s2s^1S_0 \rightarrow 1s^21S_0$ transition in He-like ions.

| Isotope | Z  | I  | $\mu_I$ | $\lambda$ (Å) | $A_{HIT}$ |
|---------|----|----|---------|----------------|-----------|
| $^{12}$C | 6  | 1/2 | 0.7042  | 40.7306        | 40.7304   | 2.6704[-8] |
| $^{19}$F | 9  | 1/2 | 2.628868| 16.9361        | 16.9404   | 1.0862[-4] |
| $^{28}$Si | 14 | 1/2 | -0.55529| 6.6835        | 6.6848    | 2.4515[-3] |
| $^{47}$Ti | 22 | 5/2 | -0.78848| 2.6214        | 2.6225    | 1.3010[0]  |
| $^{57}$Fe | 26 | 1/2 | 2.56277 | 1.8584        | 1.8594    | 3.7865[-1] |
| $^{70}$Ga | 31 | 3/2 | 2.6289  | 1.2940        |           | 1.9830[3]  |
| $^{85}$Rb | 37 | 5/2 | 1.35298 | 0.8987        |           | 5.5705[3]  |
| $^{97}$Mo | 42 | 5/2 | -0.9335 | 0.6916        | 0.6923    | 1.5643[4]  |
| $^{103}$Rh | 45 | 1/2 | -0.884  | 0.5994        |           | 7.9312[4]  |
| $^{117}$Sn | 50 | 1/2 | -1.00104| 0.4814        | 0.4820    | 4.4904[5]  |
| $^{131}$Xe | 54 | 3/2 | 0.6908  | 0.4098        | 0.4104    | 3.5374[5]  |
| $^{151}$Eu | 63 | 5/2 | 3.4717  | 0.2958        |           | 6.7634[7]  |
| $^{175}$Lu | 71 | 7/2 | 2.2323  | 0.2289        |           | 1.4508[8]  |
| $^{193}$Ir | 77 | 3/2 | 0.1637  | 0.1917        |           | 3.3463[6]  |
Figure 2: Logarithm of hyperfine induced rates $A_{HT}$ for the $1s2s^1S_0 \rightarrow 1s^2 {^1}S_0$ transition of He-like ions together with fit to the corresponding electronic quantity $A^{el}$. 