Journal of
Thai Interdisciplinary Research
Volume 14, Number 2, Pages 58 – 61

Forbidden transitions (E2, M1 and M2) in Mg-like gold

Gülay Günday Konan* **and Leyla Özdemir**

Physics Department, Sakarya University, Sakarya 54187, Turkey

Abstract

In this work, forbidden transition (E2, M1 and M2) parameters were investigated. These include wavelengths, weighted oscillator strengths and transition probabilities for Mg-like Au (Au^{67+}). Investigations were carried out using the AUTOSTRUCTURE atomic code developed by Badnell [7]. Quantum electrodynamics (QED) and relativistic effects (Breit) calculations were carried out. Correlation effects were also considered. The results obtained have been compared with existing literature and show a good match.

Keywords: forbidden transitions, transition probabilities, weighted oscillator strengths
Article history: Received 30 June 2018, Accepted 19 April 2019

1. Introduction

Many research projects and technological areas such as astrophysics, plasma physics, thermonuclear fusion, and isotope separation by lasers require accurate atomic structure and spectral data [1]. Atomic radiative transitions are important, especially in plasmas and astrophysics. The largest transition probability (or rates) is general, for electric dipole (E1) radiation, dominated by the least factor $1/\alpha^2$ over other types of transitions (E2, E3, M1, M2, etc.). Therefore E1 transitions are referred 'allowed' whereas higher order electric and all magnetic transitions are called as 'forbidden'. The data for the analysis of forbidden lines (E2, M1, M2, etc.) in the spectrum is important for the study of the plasma in astrophysical objects and fusion devices. In addition to this, it is well known that highly-charged ions are of great interest in the study of fusion energy devices [2] and in astronomy [3]. Several works for the atomic structure of magnesium (Mg) like gold exist in the literature. However, the works dealing with forbidden lines of Mg like gold are limited [4-6].

In this work wavelengths, λ (in Å), weighted oscillator strengths, gf and transition probabilities (or rates) Ar (in s^{-1}) for forbidden lines in Mg-like gold (Au^{67+}, Z = 79) are presented. These were investigated using the AUTOSTRUCTURE code developed by Badnell [7]. For this study the following configurations were selected; $2p^6 3snl$ ($n = 3-6, l = 0-4$), $2p^6 3pnl$ ($n = 3-4, l = 0-3$), $2p^6 3p5s$, $2p^6 3dnl$ ($n = 3-4, l = 0-3$), $2p^5 3s^2 3p$, $2p^5 3s 3p^2$, $2p^5 3p^3$, $2p^5 3s^2 3d$, $2p^5 3s^2 4s$, $2p^5 3s 3p 3d$, $2p^5 3p^2 3d$, $2p^5 3d^3$, $2p^5 3s 3d^2$ and $2p^5 3s 3p 4s$.

2. Calculation Method

AUTOSTRUCTURE code [7, 8] is a general program for the calculation of atomic and ionic energy levels, radiative and autoionization rates and photoionization cross sections using non-relativistic or semi-relativistic wavefunctions. It is based on SUPERSTRUCTURE [9]. In this code, the configuration set can be chosen and new configurations can be added to improve accuracy (a configuration interaction expansion, CI expansion). The CI expansion is related to the choice of radial functions. Each (nl) radial function is calculated using the Thomas-Fermi or Slater-type-orbital potential model. The Hamiltonian in any coupling model (LS, IC, or ICR) is diagonalized to obtain eigenvalues and eigenvectors. These can then be used to construct the rates. Quantum electrodynamics (QED) contributions include vacuum polarization and self-energy contributions to level energies. The finite nucleus effect is taken into account by assuming an extended Fermi distribution for the nucleus. Both of Breit and QED contributions are treated as perturbation. More detailed information on the method of the code can be found in the literature [7, 8, 10].

*Corresponding author; email: ggunday@sakarya.edu.tr

DOI 10.14456/jtir.2019.20

Table 1. Wavelengths, λ (Å), weighted oscillator strengths, gf, and transition probabilities (or rates), Ar(s^{-1}), for some forbidden lines (E2, M1, M2) in Mg-like gold (Au^{67+}). Numbers in brackets represent powers of 10.We have omitted the core $1s^2 2s^2 2p^6$ in the table.

Upper Level	J	Lower Level	J	λ (Å) This Work	λ (Å) Other Works	*gf* This Work	*gf* Other Works	Ar(s^{-1}) This Work	Ar(s^{-1}) Other Works
E2 Transitions									
$3s_{1/2}3p_{3/2}$	2	$3s_{1/2}3p_{1/2}$	0	24.53	24.597 [a]	4.62(-6)	-	1.02(7)	9.97(6) [a]
$3s_{1/2}3p_{3/2}$	2	$3s_{1/2}3p_{3/2}$	1	25.45	25.470 [a]	6.73(-6)	-	1.38(7)	1.36(7) [a]
$3d_{5/2}4f_{5/2}$	2	$3p_{1/2}3d_{5/2}$	2	2.99	3.0567 [b]	5.39(-3)	1.40(-3) [b]	0.80(12)	1.00(12) [b]
$3p_{3/2}4f_{5/2}$	1	$3p_{1/2}3p_{3/2}$	1	2.98	3.0507 [b]	3.83(-3)	3.83(-3) [b]	9.59(11)	9.16(11) [b]
$3d_{3/2}4f_{5/2}$	1	$3p_{1/2}3d_{3/2}$	1	3.38	3.0684 [b]	4.58(-3)	3.78(-3) [b]	8.91(11)	8.94(11) [b]
$3d_{5/2}4f_{5/2}$	2	$3p_{1/2}3d_{5/2}$	2	2.99	3.0641 [b]	5.39(-3)	5.33(-3) [b]	8.06(11)	7.57(11) [b]
$3p_{3/2}4f_{5/2}$	1	$3p_{1/2}3p_{3/2}$	1	2.98	3.0539 [b]	3.83(-3)	4.88(-3) [b]	9.59(11)	6.99(11) [b]
$3d_{3/2}4f_{5/2}$	1	$3p_{1/2}3d_{3/2}$	1	3.38	3.0839 [b]	4.58(-3)	4.97(-3) [b]	8.91(11)	6.98(11) [b]
$3p_{1/2}4d_{3/2}$	1	$3s_{1/2}3p_{1/2}$	1	2.90	2.9949 [b]	2.37(-3)	2.65(-3) [b]	6.30(11)	6.56(11) [b]
$3d_{3/2}4f_{5/2}$	2	$3p_{1/2}3d_{3/2}$	2	3.37	3.0458 [b]	4.23(-3)	5.81(-3) [b]	4.97(11)	5.97(11) [b]
$3d_{5/2}4d_{3/2}$	3	$3s_{1/2}3d_{5/2}$	3	2.92	2.9929 [b]	3.77(-3)	2.36(-3) [b]	4.21(11)	5.85(11) [b]
$3p_{3/2}4d_{3/2}$	2	$3s_{1/2}3p_{3/2}$	2	2.91	2.9797 [b]	2.99(-3)	2.31(-3) [b]	4.72(11)	5.79(11) [b]
$3d_{3/2}4d_{5/2}$	1	$3s_{1/2}3d_{3/2}$	1	2.88	2.9614 [b]	2.39(-3)	2.21(-3) [b]	6.41(11)	5.61(11) [b]
$3p_{3/2}4d_{5/2}$	1	$3s_{1/2}3p_{3/2}$	1	2.92	2.9701 [b]	2.74(-3)	2.22(-3) [b]	7.14(11)	5.61(11) [b]
M1 Transitions									
$3s_{1/2}3p_{3/2}$	2	$3s_{1/2}3p_{3/2}$	1	25.45	25.470 [a]	6.73(-6)	-	5.75(8)	5.59(8) [a]
$3p_{1/2}4p_{1/2}$	0	$3p_{1/2}3p_{3/2}$	1	3.10	3.9029 [b]	0	7.09(-6) b	2.42(9)	3.11(9) [b]
$3p_{3/2}4p_{3/2}$	0	$3p_{1/2}3p_{3/2}$	1	3.77	3.1813 [b]	0	2.52(-6) b	2.51(9)	1.66(9) [b]
$3d_{5/2}4p_{1/2}$	2	$3p_{3/2}3d_{5/2}$	2	3.11	3.9206 [b]	6.69(-4)	1.35(-5) [b]	1.14(9)	1.18(9) [b]
$3p_{3/2}4p_{3/2}$	3	$3p_{1/2}3p_{3/2}$	2	3.13	3.2025 [b]	3.61(-4)	1.27(-5) [b]	1.63(9)	1.18(9) [b]
$3d_{5/2}4p_{1/2}$	3	$3p_{3/2}3d_{5/2}$	3	3.13	3.9397 [b]	8.10(-4)	1.54(-5) [b]	1.25(9)	9.45(8) [b]
$3d_{5/2}4p_{1/2}$	2	$3p_{3/2}3d_{5/2}$	1	3.14	3.9634 [b]	3.10(-4)	1.05(-5) [b]	1.13(9)	8.91(8) [b]
$3p_{3/2}4d_{3/2}$	3	$3p_{3/2}3d_{5/2}$	4	3.77	3.9516 [b]	2.26(-4)	1.25(-5) [b]	1.80(8)	7.62(8) [b]
$3s_{1/2}4p_{3/2}$	1	$3s_{1/2}3p_{1/2}$	1	3.81	3.1955 [b]	1.14(-3)	2.48(-6) [b]	4.55(8)	5.40(8) [b]
$3s_{1/2}4p_{1/2}$	1	$3s_{1/2}3p_{3/2}$	1	3.11	3.9450 [b]	6.35(-4)	3.61(-6) [b]	7.31(8)	5.17(8) [b]
M2 Transitions									
$3s_{1/2}3p_{3/2}$	2	3s2	0	18.79	18.803 [a]	0	-	7.25(5)	7.37(5) [a]
$3s_{1/2}3p_{3/2}$	2	$3p_{1/2^2}$	0	44.93	42.781 [a]	0	-	7.41(1)	7.51(1) [a]
$3d_{3/2}4f_{7/2}$	5	$3d_{3/2}3d_{5/2}$	4	3.72	3.8462 [b]	8.90(-7)	7.95(-5) [b]	4.75(9)	3.26(9) [b]
$3d_{5/2}4f_{5/2}$	5	$3d_{5/2^2}$	4	3.82	3.8192 [b]	9.88(-7)	6.21(-5) [b]	2.73(9)	2.58(9) [b]
$3d_{5/2}4f_{7/2}$	6	$3d_{5/2^2}$	4	3.85	3.8495 [b]	4.54(-6)	6.30(-5) [b]	2.22(9)	2.18(9) [b]
$3d_{3/2}4f_{7/2}$	5	$3d_{3/2}3d_{5/2}$	3	3.71	3.8274 [b]	1.24(-6)	2.20(-5) [b]	1.01(9)	9.10(8) [b]
$3d_{5/2}4f_{5/2}$	0	$3d_{3/2}3d_{5/2}$	2	3.72	3.7247 [b]	0	1.16(-6) [b]	6.01(8)	5.59(8) [b]
$3d_{5/2}4f_{7/2}$	6	$3d_{3/2}3d_{5/2}$	4	3.72	3.7318 [b]	1.78(-6)	1.39(-5) [b]	5.54(8)	5.11(8) [b]
$3d_{5/2}4f_{7/2}$	5	$3d_{3/2}3d_{5/2}$	3	3.82	3.6859 [b]	2.50(-6)	1.14(-5) [b]	2.01(8)	5.09(8) [b]

[a]Ref. [4], [b]Ref. [6]

Inbuilt into the code is the following theory. If the emitted or observed photon has angular momentum k and parity, $\pi = (-1)^k$, the transition is an electric multipole transition (E^k). If the transition is from an absorbed photon with parity$\pi = (-1)^{k+1}$, it is a magnetic multipole transition (M^k). The transition probability for the emission from the upper level to the lower level is given by

$$A^{\pi k}(\gamma' J', \gamma J) = 2C_k\left[\alpha\left(E_{\gamma' J'} - E_{\gamma J}\right)\right]^{2k+1} \frac{S^{\pi k}(\gamma' J', \gamma J)}{g_{J'}} \quad (1)$$

where $S^{\pi k}$is line strength and can be found using the following,

$$S^{\pi k}(\gamma' J', \gamma J) = \left|\left\langle \gamma J \| \mathbf{O}^{\pi(k)} \| \gamma' J' \right\rangle\right|^2 \quad (2)$$

and $C_k = (2k+1)(k+1)/k((2k+1)!!)^2$, and $\mathbf{O}^{\pi(k)}$ is transition operator.

The weighted oscillator strength (or gf-value) is like the line strength between two levels,

$$gf^{\pi k}(\gamma' J', \gamma J) = g_{J'} f^{\pi k}(\gamma' J', \gamma J) \quad (3)$$

where $g_{J'}$ denotes statistical weight of the upper level, namely $g_{J'} = 2J' + 1$.

3. Results and Discussion

In this work, the electric quadrupole (E2), magnetic dipole (M1) and magnetic quadrupole (M2) transition parameters were analysed. Wavelengths, λ (in Å), weighted oscillator strengths, gf and transition probabilities (or rates) Ar (in s^{-1}) have been reported for some levels in Mg-like gold (Au^{67+}, Z = 79) using the AUTOSTRUCTURE code developed by Badnell [7]. The ground-state configuration of Au^{67+} is [Ne] $3s^2$. This was taken into account in the configurations which included valence-valence and core-valence correlations to calculate atomic structure properties: $2p^6 3snl$ ($n = 3-6, l = 0-4$), $2p^6 3pnl$ ($n = 3-4, l = 0-3$), $2p^6 3p5s$, $2p^6 3dnl$ ($n = 3-4, l = 0-3$), $2p^5 3s^2 3p$, $2p^5 3s 3p^2$, $2p^5 3p^3$, $2p^5 3s^2 3d$, $2p^5 3s^2 4s$, $2p^5 3s 3p 3d$, $2p^5 3p^2 3d$, $2p^5 3d^3$, $2p^5 3s 3d^2$, $2p^5 3s 3p 4s$. In calculations, the quantum electrodynamics (QED) and relativistic Breit interactions were considered in addition to correlation effects. As the nuclear charge increases, relativistic and QED corrections grow rapidly. For this reason it is important that relativistic and QED corrections were considered.

Table 1 shows the wavelengths, λ (in Å), weighted oscillator strengths gf and transition rates Ar (in s^{-1}) for forbidden transitions (E2, M1, and M2). It also shows the comparison of the results from this study with available literature [4, 6]. This table only includes a part of the forbidden transition results obtained from this work. In the table, the number in brackets represents the power of 10. The core $1s^2 2s^2 2p^6$ has been omitted in the table, and the states that are displayed are in intermediate coupling.

Energy levels and E1 transitions for Mg like gold were reported in previous work by the author [11]. In this paper part of our forbidden transition results is presented and are compared with the results of other works [4, 6] in the literature. The electric quadrupole (E2), magnetic dipole (M1) and magnetic quadrupole (M2) transition parameters that were found agreed with other works with the exception of some levels. Although wavelengths (λ) and transition rates (Ar) have good agreement, the weighted oscillator strengths (gf) were found to be a little different from the other works. It is thought that these cases occured due to some restrictions in the two methods that were used. It is thought that these methods could be improved through use of configurations which include more core-core correlations. In our work this was not possible as the program procedure doesn't run because of the huge number of levels that would then require analysis. One other shortcoming of our work was that the gf of some transitions were found to be zero. This was due to the fact that values less than 10^{-6} have been were automatically reduced to zero by the code. Our results generally agree with [4] although. The transitions between low levels show the best agreement. It should be noted that our results and those obtained by others need to compare with real experimental results in order to assess their real life accuracy

4. Conclusion

The aim of this work was to investigate forbidden transitions parameters which are useful in analyzing of the spectrum of Mg like gold. It is well known that the accurate radiative transition rates are required. This is particularly the case for astrophysical plasmas. This paper has presented e-atomic data which is sufficiently accurate for Au plasma diagnostics and modeling, as well as various other atomic and astrophysics applications.

Acknowledgements

This work was supported by Research Fund of the Sakarya University (Project Number: 2013-50-02-013).

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