Turkish Computational and Theoretical Chemistry

Turkish Comp Theo Chem (TC&TC)

Volume(Issue): 2(2) – Year: 2018 – Pages: 1-6

ISSN: 2587-1722 / e-ISSN: 2602-3237

Received: 20.02.2018 ***Accepted***: 18.04.2018 *Research Article*

Radiative transition probabilities for levels of $3p^63d^2$- $3p^53d^3$ transitions in W^{54+}

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Abstract: We have reported the electric dipole (E1), magnetic dipole (M1) and electric quadrupole (E2) transition probabilities for some levels of $3p^63d^2$ and $3p^53d^3$ in Ca-like tungsten ion (W^{54+}) using the AUTOSTRUCTURE code, which uses non-relativistic or kappa-averaged relativistic wave functions and the full Breit interaction in the Pauli approximation. In calculations, quantum electrodynamical (QED) contributions and correlation effects have been also taken into account. The results obtained have been compared with the available experimental and theoretical results.

Keywords: *Radiative transition, Transition probabilities, QED, Correlation.*

1. Introduction

Spectral data of highly ionized tungsten ions play an important role in different areas such as plasma science, fusion reaction, high energy astrophysics and biomedical applications. For example it hold a special place in future magnetic confinement fusion reactors such as the ITER because of its desirable properties with low hydrogen retention, high melting point, and high thermal conductivity [1].

A number of works dealing with the transiton rates (or probabilities) of Ca-like W exist in the literature. Safronova and Safronova [2] tabulated wavelengths and transition probabilities for *nl–n'l'* transitions in W^{54+} ion. Wavelengths and transition probabilities were calculated for forbidden lines of $3p^63d^2$ ground configurations of W^{54+} ion by Quinet [3]. Guo et al. [4] reported relativistic many body calculations on wavelengths and transition probabilities for forbidden transitions among the levels belong to ground state configuration in Ca-like tungsten. Extensive self-consistent multi-configuration Dirac-Hartree-Fock (MCDHF) calculations were performed for the $3p^63d^2$ ground configurations of W^{54+} ion by Zhao et al. [5]. Ding et al. calculated radiative transition parameters for W^{54+} ion comprehensively [6-9]. All these works are theoretical. On the experimental side, Ralchenko et al. [10,11] measured extreme ultraviolet (EUV) spectra of highly charged tungsten ions, including W^{54+} ion, using an electron-beam ion trap (EBIT).

In this work we have calculated transition probabilities for the electric dipole (E1), electric quadrupole (E2), and magnetic dipole (M1) transitions in Ca-like tungsten (W^{54+}) using the AUTOSTRUCTURE code [12]. Calculations include quantum electrodynamics (QED) (self-energy and vacuum polarization) and Breit interaction (magnetic interaction between the

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electrons and retardation effects of the electron-electron interaction) contributions. These contributions are important in investigations include electronic structure and spectroscopic properties of many electron systems. We have taken into account the configurations of *$3p^63d^2$, $3p^63d4s$, $3p^63d4p$, $3p^63d4d$, $3p^63d4f$, $3p^63d5s$, $3p^63d5p$, $3p^64s^2$, $3p^64s4p$, $3p^64s4d$, $3p^64s4f$, $3p^64p^2$, $3p^64p4d$, $3p^64p4f$, $3p^64d^2$, $3p^65s^2$, $3p^65s5p$, $3p^65s5d$, $3p^53d^3$, $3p^53d^24s$, $3p^53d4s4d$, $3p^54s^24p$, $3p^54s4p^2$, $3p^54p^3$, $3p^54s^24d$, $3p^53d4s4p$, $3p^43d^34s$*.

2. Calculation Method

AUTOSTRUCTURE code [12] 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 wave functions. It is based on SUPERSTRUCTURE [13]. In this code, the configuration set is chosen optionally and added new configuration 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 in 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 with which to construct the rates. Detailed information on the method of this code can be found in [13-15].

Radiative properties of atoms are described with on electromagnetic transition between two states, characterized by the angular momentum and parity of the corresponding photon [16]. If the emitted or observed photon has angular momentum k and parity, $\pi = (-1)^k$, the transition is an electric multipole transition (E^k), while the transition from absorbed the photon with parity $\pi = (-1)^{k+1}$, is magnetic multipole transition (M^k). The transition probability for the emission from the upper level to the lower level is given by

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

where $S^{\pi k}$ is line strength,

$$S^{\pi k}\left(\gamma' J',\gamma J\right) = \left|<\gamma J \parallel \mathbf{O}^{\pi(k)} \parallel \gamma' J'>\right|^2 \qquad (2)$$

and $C_k = (2k+1)(k+1)\big/k((2k+1)!!)^2$, and $\mathbf{O}^{\pi(k)}$ is transition operator. The weighted oscillator strength (or *gf*-value) is

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

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

3. Results and Discussion

In this work, transition probabilities (or rates) have been reported for the electric dipole (E1), electric quadrupole (E2), and magnetic dipole (M1) transitions in Ca-like tungsten (W^{54+}) using the AUTOSTRUCTURE code [12]. In calculations quantum electrodynamical (QED) contributions and Breit corrections and various correlation (valence and core-valence and core-core) effects have been taken into account. Therefore we have considered *$3p^63d4l$ (l=0-3), $3p^64l4l'$ (l=0-1 and l'=0-3), $3p^63d5s$, $3p^63d5p$, $3p^64d^2$, $3p^65s^2$, $3p^65s5p$, $3p^65s5d$, $3p^53d^3$, $3p^53d^24s$, $3p^53d4s4d$, $3p^54s^24p$, $3p^54s4p^2$, $3p^54p^3$, $3p^54s^24d$, $3p^53d4s4p$, $3p^43d^34s$* configurations in the calculations. The ground state configuration of W^{54+} is [Ne]$3s^23p^63d^2$. In the tables, the core of $1s^22s^22p^63s^2$ is omitted and the number in brackets represents the power of 10.

We have obtained 466 transitions for electric dipole transitions between $3p^63d^2$ and $3p^53d^3$ levels. The E1 transition probabilities, A_r, (in s^{-1}), in particular for low lying levels, have been briefly given in Table 1. In Fig. 1, all transitions have been used. The obtained results have been here compared with the results from multi-configuration Dirac-Fock (MCDF) [9]. In Figure 1, we have shown the comparison between our transition probabilities and those reported by Ding et al. [9] for all $3p^63d^2$ - $3p^53d^3$ transitions. As seen from Figure 1, the transition probabilities obtained from our calculations are in good agreement with [9] except $3p^63d^2\ {}^1G_4$ - $3p^53d^3\ {}^3I_5$ and $3p^63d^2\ {}^1D_2$ - $3p^53d^3\ {}^3D_3$ transitions.

Table 1. Transition probabilities, A_r (s^{-1}), for electric dipole (E1) transitions in $3p^63d^2$ - $3p^53d^3$ for Ca-like tungsten (W^{54+})

Levels				This work	Other works
Lower		Upper		A.S.	MCDF^a
$3p^63d^2$	$^3P_0$	$3p^53d^3$	$^3D_1$	9.19(11)	9.33(11)
$3p^63d^2$	$^3F_2$	$3p^53d^3$	$^3D_1$	2.88(11)	2.95(11)
$3p^63d^2$	$^3P_1$	$3p^53d^3$	$^3P_0$	1.40(12)	1.15(12)
$3p^63d^2$	$^3F_4$	$3p^53d^3$	$^3D_3$	1.40(12)	1.16(12)
$3p^63d^2$	$^1G_4$	$3p^53d^3$	$^1F_3$	1.36(12)	1.16(12)
$3p^63d^2$	$^1D_2$	$3p^53d^3$	$^1F_3$	1.70(12)	1.61(12)
$3p^63d^2$	$^3P_2$	$3p^53d^3$	$^3F_3$	2.42(12)	1.93(12)
$3p^63d^2$	$^3F_3$	$3p^53d^3$	$^3F_3$	2.42(12)	1.96(12)
$3p^63d^2$	$^3F_4$	$3p^53d^3$	$^3D_3$	1.90(12)	2.15(12)

^{a}[9]

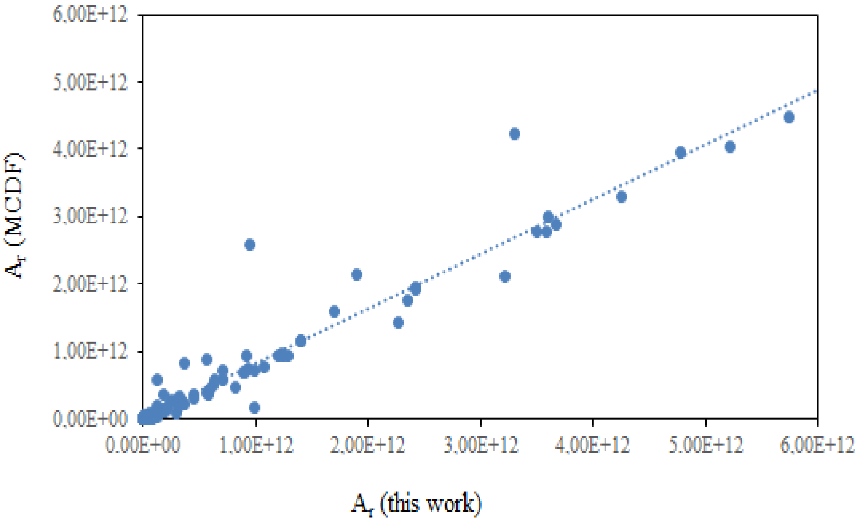

Fig. 1. Comparison of the E1 transition probabilities obtained present AUTOSTRUCTURE calculations with MCDF results [9].

The forbidden transitions, such as electric quadrupole (E2) and magnetic dipole (M1) transitions have been calculated. We have obtained 4336 forbidden transitions (E2 and M1) between $3p^63d^2$ and $3p^53d^3$ levels. The E2 and M1 transition probabilities obtained between $3p^63d^2$ levels are given in Table 2 and Table 3, respectively. We have compared E2 transition probabilities with the relativistic many body perturbation theory (RMBPT) [2] and MCDF results [9]. Our results are in agreement with other works [2, 9] except some transitions. There is also this case within the other results from MCDF and RMBPT. In Figure 2, we have shown the comparison between our E2 transition probabilities and those reported by Ding et al. [9] for the transitions between $3p^53d^3$ levels. As seen from Table 2 and Figure 2, the E2 transition probabilities obtained from our calculations are in good agreement with [9] generally.

Table 2. Transition probabilities, A_r (s^{-1}), for electric quadrupole (E2) transitions in $3p^63d^2$ ground state configuration for Ca-like tungsten (W^{54+})

Levels				**This work**	**Other works**	
Lower		**Upper**		**A.S.**	**RMBPT**[a]	**MCDF**[b]
$3p^63d^2$	$^3F_2$	$3p^63d^2$	$^3F_3$	1.48(02)	1.15(02)	1.23(02)
$3p^63d^2$	$^3F_2$	$3p^63d^2$	$^3P_2$	9.04(02)	7.31(02)	7.22(02)
$3p^63d^2$	$^3F_2$	$3p^63d^2$	$^1G_4$	5.37(02)	3.21(02)	4.61(02)
$3p^63d^2$	$^3F_2$	$3p^63d^2$	$^3P_1$	1.11(03)	1.17(03)	9.71(02)
$3p^63d^2$	$^3F_2$	$3p^63d^2$	$^3F_4$	3.02(02)	4.30(02)	3.09(02)
$3p^63d^2$	$^3F_2$	$3p^63d^2$	$^1D_2$	1.33(01)	4.50(01)	9.31(01)
$3p^63d^2$	$^3F_3$	$3p^63d^2$	$^3P_2$	1.14(02)	2.14(02)	1.16(02)
$3p^63d^2$	$^3F_3$	$3p^63d^2$	$^1G_4$	6.22(03)	4.23(05)	2.83(03)
$3p^63d^2$	$^3F_3$	$3p^63d^2$	$^3P_1$	8.05(01)	9.07(01)	8.37(01)
$3p^63d^2$	$^3F_3$	$3p^63d^2$	$^3F_4$	8.62(01)	6.13(01)	7.20(01)
$3p^63d^2$	$^3F_3$	$3p^63d^2$	$^1D_2$	1.25(03)	1.05(03)	1.06(03)
$3p^63d^2$	$^3P_2$	$3p^63d^2$	$^1G_4$	1.16(03)	8.12(04)	2.01(04)
$3p^63d^2$	$^3P_2$	$3p^63d^2$	$^3P_1$	2.36(03)	3.73(03)	2.88(03)
$3p^63d^2$	$^3P_2$	$3p^63d^2$	$^3F_4$	2.25(02)	6.29(01)	1.74(02)
$3p^63d^2$	$^3P_2$	$3p^63d^2$	$^1D_2$	1.23(02)	7.53(01)	1.23(02)
$3p^63d^2$	$^1G_4$	$3p^63d^2$	$^3F_4$	4.04(02)	4.54(02)	3.49(02)
$3p^63d^2$	$^1G_4$	$3p^63d^2$	$^1D_2$	1.05(00)	1.99(01)	4.85(00)
$3p^63d^2$	$^3P_1$	$3p^63d^2$	$^1D_2$	4.28(02)	4.18(02)	3.54(02)
$3p^63d^2$	$^3F_4$	$3p^63d^2$	$^1D_2$	2.21(02)	3.37(02)	2.94(02)

[a][2]; [b] [9]

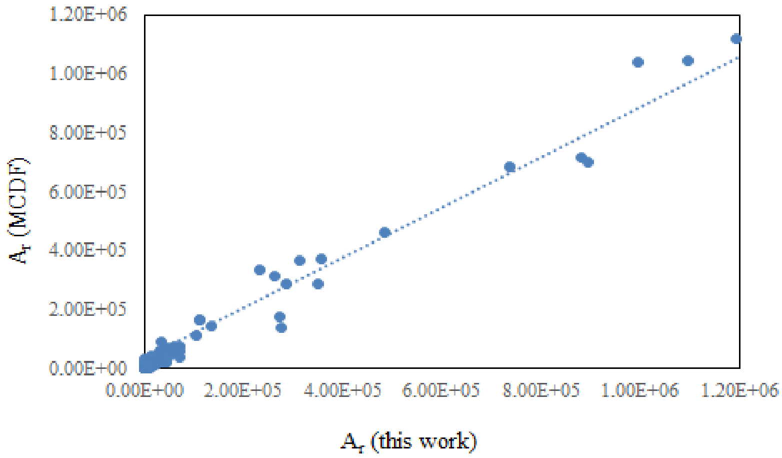

Fig. 2. Comparison of the E2 transition probabilities obtained present AUTOSTRUCTURE calculations with MCDF results [9].

We have compared M1 transition probabilities between $3p^63d^2$ levels with the (RMBPT) [2,4] and MCDF results [3,9] in Table 3. Our results are in agreement with other theoretical works [2-4,9] except $3p^63d^2$ $^3F_3$ - $3p^63d^2$ $^1G_4$ transition. There is only one experimental work in the literature [11] and our results have good agreement with these values. In Figure 3, we have shown the comparison between our M1 transition probabilities and those reported by Ding et al. [9] for the transitions between $3p^53d^3$ levels. As seen from Table 3 and Figure 3, the M1 transition probabilities obtained from our calculations are in good agreement with [9] generally.

We have listed only a part of calculation results in tables. But all figures include all results. Other results tabulated can be taken from G. Günday Konan.

Table 3. Transition probabilities, A_r (s^{-1}), for magnetic dipole (M1) transitions in $3p^63d^2$ ground state configuration for Ca-like tungsten (W^{54+})

Levels				**This work**	**Other works**		
Lower		**Upper**		**A.S.**	**RMBPT**	**MCDF**	**Exp.**
$3p^63d^2$	$^3F_2$	$3p^63d^2$	$^3F_3$	3.86(06)	3.68(06)[a] 3.64(06)[b]	3.69(06)[c] 3.68(06)[d]	3.68(06)[e]
$3p^63d^2$	$^3F_2$	$3p^63d^2$	$^3P_2$	1.89(06)	1.79(06)[a] 1.77(06)[b]	1.81(06)[c] 1.81(06)[d]	1.81(06)[e]
$3p^63d^2$	$^3F_2$	$3p^63d^2$	$^3P_1$	2.73(05)	2.58(05)[a]	2.63(05)[c]	-
$3p^63d^2$	$^3F_2$	$3p^63d^2$	$^1D_2$	1.31(04)	1.27(04)[a]	1.17(04)[c]	-
$3p^63d^2$	$^3P_0$	$3p^63d^2$	$^3P_1$	1.81(06)	1.77(06)[a] 1.71(06)[b]	1.73(06)[c] 1.74(06)[d]	1.72(06)[e]
$3p^63d^2$	$^3F_3$	$3p^63d^2$	$^3P_2$	4.19(03)	4.35(03)[a]	4.43(03)[c]	-
$3p^63d^2$	$^3F_3$	$3p^63d^2$	$^1G_4$	1.15(04)	8.55(03)[a]	8.61(03)[c]	-
$3p^63d^2$	$^3F_3$	$3p^63d^2$	$^3F_4$	4.02(06)	3.75(06)[a]	3.83(06)[c] 3.82(06)[d]	-
$3p^63d^2$	$^3F_3$	$3p^63d^2$	$^1D_2$	7.96(05)	7.52(05)[a]	7.59(05)[c]	-
$3p^63d^2$	$^3P_2$	$3p^63d^2$	$^3P_1$	5.40(02)	6.78(02)[a]	6.50(02)[c]	-
$3p^63d^2$	$^3P_2$	$3p^63d^2$	$^1D_2$	3.28(06)	3.09(06)[a]	3.12(06)[c] 3.11(06)[d]	-
$3p^63d^2$	$^1G_4$	$3p^63d^2$	$^3F_4$	1.13(06)	1.11(06)[a]	1.10(06)[c] 1.09(06)[d]	-
$3p^63d^2$	$^3P_1$	$3p^63d^2$	$^1D_2$	1.38(06)	1.28(06)[a]	1.31(06)[c] 1.30(06)[d]	-
$3p^63d^2$	$^3P_1$	$3p^63d^2$	$^1S_0$	8.39(06)	7.32(06)[a]	7.88(06)[c] 7.83(06)[d]	-

[a][2], [b][4], [c][9], [d][3], [e][11]

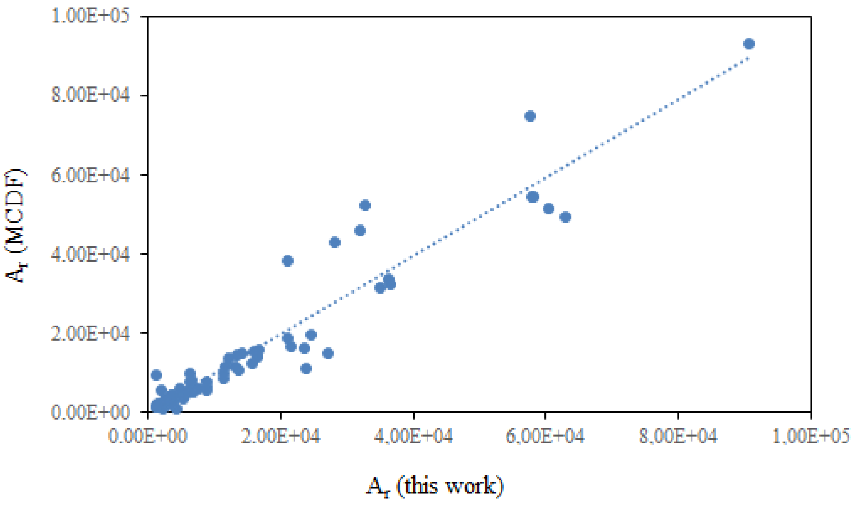

Fig. 3. Comparison of the M1 transition probabilities obtained present AUTOSTRUCTURE calculations with MCDF results [9].

4. Conclusion

In conclusion, tungsten ions are important in particular in tokamak plasmas such as ITER (International Thermonuclear Experimental Reactor fusion plasmas). In addition accurate transition probabilities are essential for quantitative spectroscopy in many fields, particularly in astrophysics and especially forbidden lines are used in plasma diagnostics due to the corresponding radiation intensities are often very sensitive to electron temperature and density. In this context transition probabilities for Ca-like tungsten must be determined with high confidence. Consequently, we hope that the results obtained from this work will be useful in analyzing of the spectrum of Ca-like tungsten ion.

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