E1, M1, E2 transition energies and probabilities of W$^{54+}$ ions

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Abstract
A comprehensive theoretical study of the E1, M1, E2 transitions of a Ca-like tungsten ion is presented. Using the multi-configuration Dirac–Fock (MCDF) method with a restricted active space treatment, the wavelengths and probabilities of the M1 and E2 transitions between the multiplets of the ground state configuration ([Ne]3s$^2$3p$^6$3d$^2$) and of the E1 transitions between [Ne]3s$^2$3p$^6$3d$^3$ and [Ne]3s$^2$3p$^6$3d$^2$ have been calculated. The results are in reasonable agreement with available experimental data. The present E1 and M1 calculations are compared with previous theoretical values. For E2 transitions, the importance of electron correlation from 3s and 3p orbitals is pointed out. Several strong E1 transitions are predicted, which have potential advantages for plasma diagnostics.

Keywords: energy level, transition rate, Ca-like tungsten ions, MCDF

1. Introduction

Tungsten (W) has become the focus of attention in fusion research, being considered as the main candidate for the cover of the plasma-facing component in next-generation fusion devices like ITER (International Thermonuclear Experimental Reactor Tokamak); tungsten has excellent physical and chemical properties such as high sputtering threshold energy, low sputtering yield, high re-deposition efficiency and low tritium retention [1, 2]. However, tungsten impurity ions are produced due to the interaction between the edge plasma and cover material. These ions may be transported to the fusion core plasmas, and be further ionized to produce highly charged W ions. These ions could cause a large radiation loss by emitting high energy photons, which leads to plasma disruption if the relative concentration of W ion impurities in the core plasma is higher than about 10$^{-8}$ [3]. Monitoring and controlling the flux of these highly charged W impurity ions are important to retain the fusion [4]. Thus, it is indispensable to carry out a comprehensive theoretical investigation on the atomic structures and transition properties of various tungsten ions.

During recent decades, several studies have been performed to provide the theoretical and experimental values of W$^{54+}$ ions [5–12]. Safronova et al calculated the magnetic dipole (M1) and electric quadrupole (E2) transitions between the multiplets of the ground state configuration ([Ne]3s$^2$3p$^6$3d$^2$) of W$^{54+}$ using the relativistic many-body perturbation theory (RMBPT) [7]. Ralchenko et al observed the M1 lines from 3d$^9$ (n = 1–9) ground state fine structure multiplets of tungsten ions with electron-beam ion trap (EBIT) and they employed a non-Maxwellian collisional-radiative model to analyze the observed spectrum [8]. Quinet calculated the forbidden transitions within the 3p$^5$ (k = 1–5) and 3d$^n$ (n = 1–9) ground state configuration multiplets of highly charged tungsten ions (W$^{53+}$–W$^{51+}$) by the multi-configuration Dirac–Fock (MCDF) method taking into account the correlations between a restricted number of configurations [9]. Furthermore, the theoretical calculations of M1 forbidden
The minimal basis set model while other models include the electron correlation contributions in different extent. The configuration space was expanded by single (S) and double (D) substitutions.

| Model       | Inactive core | Core       | Valence | Number of CSFs |
|-------------|---------------|------------|---------|----------------|
| DF          | 1s²2s²2p⁶     | 3s²3p⁶    | 3d²     | 9              |
| 3Complex    |               |            |         |                |
| Ground state configuration | 4SD       |            |         | 33 117         |
|             | 5SD(5s–5d)    |            |         | 82 303         |
|             | 5SD           |            |         | 165 870        |
|             | 6SD(6s–6d)    |            |         | 261 899        |
| Excited state configuration | DF        | 1s²2s²2p⁶ | 3s²3p⁵ | 3d¹            |
|             | 3Complex      |            |         | 104            |
|             | 4SD           |            |         | 1237           |
|             | 5SD           |            |         | 197 773        |
|             | 5SD(5s–5d)    |            |         | 494 265        |

Table 1. Expansion schemes of computational models for the ground and the first excited configurations of the W⁵⁺⁺ ion. The model DF is the minimal basis set model while other models include the electron correlation contributions in different extent. The configuration space was expanded by single (S) and double (D) substitutions.

| jj-label | Lower | Upper | DF     | 3Complex | 4SD | 5SD(5s–5d) | 5SD | 6SD(6s–6d) | Other |
|----------|-------|-------|--------|----------|-----|------------|-----|------------|-------|
| (3/2,3/2)₂ | (5/2,5/2)₂ | 7.675 | 7.689 | 7.693 | 7.693 | 7.694 | 7.694 | 7.712₉     |
| (3/2,2/1)₂ | (5/2,5/2)₀ | 12.555 | 12.734 | 12.707 | 12.713 | 12.722 | 12.723 | 12.721₉     |
| (3/2,2/1)₁ | (5/2,5/2)₂ | 13.856 | 13.964 | 13.976 | 13.977 | 13.982 | 13.981 | 14.008₉     |
| (3/2,3/2)₂ | (3/2,5/2)₁ | 14.050 | 14.122 | 14.150 | 14.152 | 14.150 | 14.150 | 14.176₉     |
| (3/2,3/2)₂ | (3/2,5/2)₂ | 14.910 | 14.958 | 14.972 | 14.973 | 14.974 | 14.974 | (14.959,14.984)₉ |
| (3/2,3/2)₄ | (5/2,5/2)₄ | 15.372 | 15.346 | 15.364 | 15.363 | 15.370 | 15.369 | 15.413₉     |
| (3/2,2/1)₂ | (5/2,5/2)₂ | 15.817 | 15.824 | 15.824 | 15.824 | 15.827 | 15.827 | 15.860₉     |
| (3/2,2/1)₁ | (5/2,5/2)₂ | 16.916 | 16.880 | 16.860 | 16.858 | 16.866 | 16.865 | 16.911₉     |
| (3/2,3/2)₂ | (3/2,5/2)₃ | 17.206 | 17.112 | 17.113 | 17.112 | 17.111 | 17.110 | (17.080,17.147)₉ |
| (3/2,5/2)₄ | (5/2,5/2)₄ | 18.645 | 18.591 | 18.561 | 18.561 | 18.553 | 18.553 | 18.593₉     |
| (3/2,2/₁)₀ | (3/2,5/2)₁ | 19.410 | 19.201 | 19.234 | 19.226 | 19.220 | 19.218 | (19.177,19.281)₉ |
| (3/2,5/2)₁ | (3/2,5/2)₂ | 87.589 | 87.917 | 89.190 | 89.183 | 89.570 | 89.579 | 90.12₃     |
| (3/2,5/2)₁ | (3/2,5/2)₂ | 111.747 | 118.807 | 119.706 | 119.806 | 119.899 | 119.920 | 119.97₄     |
| (3/2,5/2)₁ | (3/2,5/2)₂ | 243.453 | 252.799 | 257.515 | 257.885 | 257.025 | 257.047 | 255.066₃     |

Table 2. Wavelengths (λ in nm) for M1 transitions of ground configuration in a Ca-like tungsten ion. DF is the Dirac–Hartree–Fock calculation, while 3Complex, 4SD, 5SD(5s–5d), 5SD and 6SD(6s–6d) include the electron correlation contributions which were described in table 1.

For the electric dipole (E1) transitions from the excited state [Ne]3s²3p⁵3d¹ to the ground state [Ne]3s²3p⁶3d² of W⁵⁺⁺ ions, measurements were carried out in the wavelength range of 26.5–43.5 Å by Lennartsson et al in an EBIT at an...
Table 3. Radiative probabilities ($A_j$ in s$^{-1}$) for M1 transitions of ground configuration in a Ca-like tungsten ion. DF is the Dirac–Hartree–Fock calculation, while 3Complex, 4SD, 5SD(5s–5d), 5SD, and 6SD(6s–6d) include the electron correlation contributions which were described in table 1. Notation $a(b)$ for transition probabilities $A_j$ means a $\times 10^b$ s$^{-1}$.

| $jj$-label | 3Complex | 4SD | 5SD(5s–5d) | 5SD | 6SD(6s–6d) | Other |
|------------|----------|------|-------------|-----|-------------|-------|
| (3/2,3/2)$^2$ | 1.254(4) | 1.133(4) | 1.173(4) | 1.173(4) | 1.154(4) | 1.153(4) | 1.276(4)$^a$ |
| (3/2,5/2)$^2$ | 8.063(6) | 7.865(6) | 7.894(6) | 7.887(6) | 7.876(6) | 7.876(6) | 7.323(6)$^a$ |
| (3/2,5/2)$^2$ | 7.663(5) | 7.593(5) | 7.598(5) | 7.598(5) | 7.589(5) | 7.589(5) | 7.524(5)$^a$ |
| (3/2,3/2)$^2$ | 2.621(5) | 2.639(5) | 2.631(5) | 2.631(5) | 2.632(5) | 2.632(5) | 2.583(5)$^a$ |
| (3/2,3/2)$^2$ | 1.811(6) | 1.818(6) | 1.815(6) | 1.815(6) | 1.815(6) | 1.798(6)$^a$ |
| (3/2,5/2)$^4$ | 3.818(6) | 3.841(6) | 3.838(6) | 3.838(6) | 3.837(6) | 3.837(6) | 3.755(6)$^a$ |
| (3/2,5/2)$^4$ | 3.125(6) | 3.128(6) | 3.128(6) | 3.128(6) | 3.126(6) | 3.126(6) | 3.095(6)$^a$ |
| (3/2,5/2)$^4$ | 1.305(6) | 1.310(6) | 1.311(6) | 1.311(6) | 1.310(6) | 1.310(6) | 1.285(6)$^a$ |
| (3/2,3/2)$^4$ | 3.656(6) | 3.698(6) | 3.698(6) | 3.698(6) | 3.698(6) | 3.698(6) | 3.683(6)$^a$ |
| (3/2,5/2)$^4$ | 1.091(6) | 1.098(6) | 1.100(6) | 1.100(6) | 1.100(6) | 1.100(6) | 1.110(6)$^a$ |
| (3/2,3/2)$^4$ | 1.700(6) | 1.742(6) | 1.736(6) | 1.737(6) | 1.738(6) | 1.739(6) | 1.771(6)$^a$ |
| (3/2,5/2)$^4$ | 9.172(3) | 9.047(3) | 8.616(3) | 8.619(3) | 8.493(3) | 8.490(3) | 8.556(3)$^a$ |
| (3/2,5/2)$^4$ | 5.399(3) | 4.552(3) | 4.447(3) | 4.437(3) | 4.430(3) | 4.428(3) | 4.351(3)$^a$ |
| (3/2,5/2)$^4$ | 7.071(2) | 6.886(2) | 6.530(2) | 6.502(2) | 6.564(2) | 6.562(2) | 6.788(2)$^a$ |

$^a$ From Sfonova and Sfonova by the RMBPT method [7].
$^b$ From Quinet by the MCDF method [9].
$^c$ From Ralchenko et al by a non-Maxwellian collisional-radiative model [8].
$^d$ From Guo et al by the RMBPT [10].

electron beam energy of 18.2 keV [11]. A collisional-radiative model was applied to explain the observed spectrum. An MCDF calculation with restricted electron correlation effects on the 3d–3p transitions was presented by Dipti et al; they also calculated the electron impact excitation cross section and polarization degree [12].

In the present work, the MCDF method with large active space is employed to calculate the E1, M1, E2 transitions for W$^{54+}$ ions. A large-scale systematic computation is carried out to fully consider various correlation effects. In previous MCDF calculations, some important correlation effects were omitted. These correlation effects are included in the present work. In the following section, a brief description of the theory that is employed in the present paper is given. In section 3, the results of the present calculation will be tabulated together with available experimental and theoretical values. The plausibility of the present theoretical method is discussed in detail. Finally, concluding remarks on the present work are given in section 4.

2. Theory and computational methodology

The MCDF method is a widely used theoretical method that is based on a relativistic atomic theory. It was presented in great detail in the monograph by Grant [13], and a number of codes based on the MCDF method were developed in the last several decades [14–16]. The present calculation employs GRASP2K package [16]. In the MCDF method, the atomic state function (ASF) $\Psi(PJM_\lambda)$ for a given state with parity $P$, total angular momentum $J$, and its z component $M_\lambda$ is represented by a linear combination of configuration state functions (CSFs) $\Phi(\gamma,PJM_\lambda)$ with the same $P, J, M_\lambda$; we have

$$\Psi(PJM_\lambda) = \sum_{i=1}^{N_c} C_i \Phi(\gamma,PJM_\lambda),$$

where $C_i$ is the mixing coefficient and $\gamma$ denotes all other quantum numbers necessary to define the configuration, $N_c$ is the number of CSFs used in the expansion. The CSFs are the linear combinations of products of members of an active
space of spin-orbitals, which are optimized simultaneously via the self-consistent field (SCF) method for the Dirac–Hartree–Fock (DHF) equation in the extended optimal level (EOL) mode. The expansion coefficients $c_i$ of the CSFs are determined variationally by optimizing the energy expectation value of the Dirac–Coulomb Hamiltonian. The Breit interaction is introduced in the low-frequency limit, and the quantum electrodynamics effects (QED) and Breit interaction effects are taken into account.

Once the atomic state functions have been calculated, the transition probability $A_{ji}$ for a multipole transition with rank $L$ from the state $J$ to $J'$, can be expressed by the reduced matrix element with the following formula:

$$A_{ji} = \frac{2\omega}{c} \frac{1}{(2L+1)(2J+1)} \left| \langle \psi_i (\gamma'J') | \hat{O}^L | \psi_i (\gamma J) \rangle \right|,$$

(2)

where $\hat{O}^L$ is a multipole radiation field operator of rank $L$.

The ground state configuration of $\text{W}^{54+}$ is $[\text{Ne}]3s^23p^63d^4$ and the first excited configuration is $[\text{Ne}]3s^23p^63d^5$. They are complex multi-electron systems and electron correlation effects should play an essential role in their structures and transition properties. In the MCDF method, electron correlation effects may be treated by building the configuration state function expansion space systematically, which is the key to evaluating the electronic correlation effects efficiently and circumventing the convergence problem that one frequently encounters in SCF calculations. In the present work, an active space (AS) approach was employed and the configuration space was expanded by single (S) and double (D) substitutions from $3s, 3p, 3d$ orbitals to a specific active set.

The present electron correlation models and the number of CSFs used to describe the ground and excited states of $\text{W}^{54+}$ ion are listed in table 1. The column ‘Model’ indicates the correlation models. DF is the Dirac–Hartree–Fock (DHF) calculation. The notation 3Complex indicates the set of all configurations in a complex within the principal quantum number $n = 3$. NSD ($N = 4, 5, 6$) represents the configuration constructed by the SD substitution from $3s, 3p, 3d$ to an AS $\{nl|n = 4, \ldots, N; l = 0, 1, \ldots, n - 1\}$. The notations $5SD(5s–5d)$ and $6SD(6s–6d)$ specify only the SD substitution into s, p and d orbitals with corresponding principal quantum number. The $3s$ and $3p$ orbitals are treated as the core, and the $3d$ orbital as the valence orbital for both ground and excited state configurations.

It has been realized in previous papers [17, 18] that the various electron correlation effects play an important role in the calculation of atomic structure from the MCDF calculation for $\text{W}^{26+}$ and $\text{W}^{27+}$ ions. In the present paper, some VV (valence–valence), CV (core–valence) and CC (core–core) correlations are included. The DHF calculation was first made for the ground and excited states. Then the configuration space was extended by increasing the active orbital set layer by layer to investigate the correlation contributions, and only the newly additional orbitals were optimized for the large active set at each step.

3. Results

3.1. M1 and E2 transitions between the ground state multiplets

The M1 transition wavelengths and probabilities between the ground state multiplets are tabulated in tables 2 and 3, respectively. The $jj$ coupling scheme is used throughout the
Table 5. Radiative probabilities \( A_j \) in \( s^{-1} \) in the Coulomb (C) and Babushkin (B) gauges for E2 transitions of ground configuration in a Ca-like tungsten ion. DF is the Dirac–Hartree–Fock calculation, while 3Complex, 4SD, 5SD(5–5d), SSD, and 6SD(6s–6d) include the electron correlation contributions which were described in Table 1. Notation a(b) for transition probabilities \( A_j \) means a \( \times 10^a \) \( (s^{-1}) \).

| \( j\ell \)-label | \( A_j \) (in \( s^{-1} \)) |
|------------------|-----------------|
|                  | Gauges          | 3Complex | 4SD        | 5SD(5s–5d) | SSD      | 6SD(6s–6d) |
| (3/2,3/2), (5/2,5/2) \( b \) | C 5.974(1) 4.651(2) 3.311(2) 5.790(2) 1.758(3) 1.816(3) | B 2.188(3) 2.344(3) 2.375(3) 2.465(3) 2.373(3) 2.386(3) |
|                  | C 1.074(2) 3.214(2) 3.435(3) 3.982(1) 7.513(1) 7.676(1) | B 1.496(1) 8.782(1) 9.062(1) 9.318(1) 8.504(1) 8.558(1) |
|                  | C 1.119(2) 6.236(2) 5.441(2) 5.517(2) 2.024(2) 2.024(2) | B 2.543(2) 3.202(2) 3.052(2) 3.092(2) 2.963(2) 2.970(2) |
|                  | C 2.490(0) 4.566(1) 3.387(1) 5.696(1) 2.304(2) 2.359(2) | B 3.882(2) 3.059(2) 2.867(2) 2.813(2) 2.878(2) 2.872(2) |
|                  | C 2.190(3) 3.405(3) 2.774(3) 3.279(3) 5.921(3) 5.996(3) | B 7.929(3) 7.061(3) 6.793(3) 6.837(3) 6.739(3) 6.749(3) |
|                  | C 9.260(2) 8.950(2) 7.420(2) 7.890(2) 9.882(2) 9.925(2) | B 1.232(3) 1.118(3) 1.061(3) 1.065(3) 1.056(3) 1.058(3) |
|                  | C 6.565(2) 6.455(2) 5.421(2) 5.934(2) 8.951(2) 9.015(2) | B 1.129(3) 1.025(3) 9.687(2) 9.718(2) 9.639(2) 9.650(2) |
|                  | C 4.669(2) 9.413(2) 7.871(2) 7.838(2) 3.709(2) 3.697(2) | B 4.522(2) 4.806(2) 4.579(2) 4.615(2) 4.535(2) 4.543(2) |
|                  | C 7.975(2) 7.514(2) 6.139(2) 6.373(2) 6.800(2) 6.814(2) | B 8.677(2) 7.618(2) 7.205(2) 7.228(2) 7.219(2) 7.226(2) |
|                  | C 8.080(1) 7.910(1) 6.564(1) 6.793(1) 6.752(1) 6.773(1) | B 7.934(1) 7.558(1) 7.182(1) 7.205(1) 7.121(1) 7.127(1) |
|                  | C 1.385(2) 1.655(2) 1.382(2) 1.394(2) 1.158(2) 1.159(2) | B 1.082(2) 1.260(2) 1.228(2) 1.239(2) 1.215(2) 1.217(2) |
|                  | C 5.728(1) 1.198(1) 1.260(2) 1.214(1) 2.021(1) 2.035(1) | B 9.374(1) 3.784(0) 4.646(0) 4.586(0) 4.388(0) 4.427(0) |
|                  | C 3.634(2) 3.708(2) 3.048(2) 3.153(2) 3.355(2) 3.364(2) | B 3.887(2) 3.682(2) 3.520(2) 3.542(2) 3.533(2) 3.538(2) |
|                  | C 1.597(2) 1.631(2) 1.336(2) 1.353(2) 1.175(2) 1.174(2) | B 1.316(2) 1.289(2) 1.232(2) 1.237(2) 1.226(2) 1.227(2) |
|                  | C 3.726(2) 2.333(2) 1.859(2) 1.840(2) 1.917(2) 1.910(2) | B 1.880(2) 1.807(2) 1.737(2) 1.742(2) 1.738(2) 1.740(2) |
|                  | C 3.900(2) 4.008(2) 3.298(2) 3.393(2) 3.297(2) 3.304(2) | B 3.772(2) 3.613(2) 3.468(2) 3.497(2) 3.485(2) 3.491(2) |
|                  | C 1.857(2) 1.610(2) 1.331(2) 1.290(2) 1.016(2) 1.013(2) | B 9.963(1) 1.031(2) 9.849(1) 9.977(1) 9.920(1) 9.944(1) |
|                  | C 3.408(2) 1.940(0) 1.573(0) 3.278(0) 1.998(1) 2.058(1) | B 3.779(1) 2.667(1) 2.619(1) 2.610(1) 2.571(1) 2.570(1) |
|                  | C 3.095(1) 1.301(0) 1.158(0) 2.189(0) 1.389(1) 1.420(1) | B 2.363(1) 1.781(1) 1.680(1) 1.677(1) 1.663(1) 1.663(1) |

* From Safronova and Safronova by the RMBPT method [7].

Paper. Notations \( \lambda \) and \( A \) are the transition wavelengths (in nm) and the transition probabilities (in \( s^{-1} \)). The meaning of the notations DF, 3Complex, 4SD, 5SD(5–5d), 5SD and 6SD(6s–6d) are given in Table 1. ‘Other’ represents the results from EBIT experiments or other theoretical work, such as the RMBPT, MCDF and RCI methods [7–10]. For the M1 transitions, the calculated wavelengths and probabilities are converged with the increase of AS and are in reasonable agreement with available experimental data. Rachenko et al [8] calculated the energy levels of the ground state and the M1 radiative transition probabilities for the \( \text{W}^{54+} \) ion by FAC. The configuration interaction among the \( n = 3 \) complex and the single excitation up to \( n = 5 \) was included in their calculation. To obtain the RMBPT results, Safronova et al [7] started their calculations from \( 1s^22s^22p^63s^23p^6 \) Dirac–Fock potential for a Ca-like tungsten ion. In the previous MCDF calculations from Quinet [9], the correlation within the \( n = 3 \) complex and some \( n = 3 \rightarrow n' = 4 \) single excitations were taken into account. In order to ensure completeness, we have included more extensively in the present calculations.

The E2 transition wavelengths \( \lambda \) (in nm) and probabilities \( A \) (in \( s^{-1} \)) in the Babushkin (B) and Coulomb (C) gauges, which correspond to the length and velocity gauge in non-relativistic theory, with values of each correlation model are given in tables 4 and 5, respectively. Some transitions from the same initial and final states could be fulfilled either by M1 or E2 transitions which were labeled with ‘*’ in.
The increase of AS. The relative deviation for most of the agree well with the theoretical results by RMBPT indicate the accuracy of the wavefunction to some extent. calculated E2 transition probabilities in different gauges from the correlation of 3s and 3p orbitals will be discussed in another paper [19].

### 3.2. E1 transitions between 3s23p53d3, with open p and d orbitals. It should be noted that the number of CSFs significantly increases with the increase of the active space, especially for the open subshell configuration with high angular momentum quantum numbers. The number of configurations for excited states ([Ne]3s23p53d4) in the 6SD(6s–6d) model is 1 651 545. It was found that an MCDF procedure for such a large scale ASF was not practically tractable with our present calculation resources. However, we found that both the energies and probabilities of M1 and E2 transitions between the ground state multiplets were almost convergent up to the calculations in the 5SD(5s–5d) and 5SD correlation models. We have assumed that the same also holds for the singly excited [Ne]3s23p3d4 configurations. Thus, we have performed the active space procedure in MCDF calculations up to the 5SD(5s–5d) correlation models for both the ground and excited state configurations.

Some E1 transition wavelengths λ (in nm) and probabilities A (in s−1) in the Coulomb (C) and Babushkin (B) gauges from [Ne]3s23p5d4 to [Ne]3s23p3d2 in different correlation models are listed in tables 6 and 7, respectively. It can be seen from these two tables that the quality of the convergence of the transition wavelengths and A-values is good. The final E1

| jj-label | λ (nm) | DF | 3Complex | 4SD | 5SD(5s–5d) | Exp. | Other |
|----------|--------|----|----------|----|------------|------|-------|
| [3p63d12]J | 2.9414 | 2.9371 | 2.9521 | 2.9530 | 2.9560 | 2.9456 | 2.9456 |
| [3p63d12]J | 3.0171 | 3.0953 | 3.1107 | 3.1115 |       |       |       |
| [3p63d12]J | 3.0898 | 3.0825 | 3.0940 | 3.0947 |       |       |       |
| [3p63d12]J | 3.0876 | 3.0756 | 3.0890 | 3.0898 |       |       |       |
| [3p63d12]J | 1.9215 | 1.9240 | 1.9265 | 1.9266 |       |       |       |
| [3p63d12]J | 1.9008 | 1.9050 | 1.9085 | 1.9086 |       |       |       |
| [3p63d12]J | 1.8508 | 1.8558 | 1.8591 | 1.8593 |       |       |       |

Table 6. Some wavelengths (λ in nm) for E1 transitions in a Ca-like tungsten ion. DF is the Dirac–Hartree–Fock calculation, while 3Complex, 4SD, 5SD(5s–5d) include the electron correlation contributions which were described in table 1.

| table 4. These E2 transition probabilities are generally by three to five orders of magnitude smaller than the M1 transition probabilities. It can be seen from tables 4 and 5 that the calculate wavelengths and probabilities are converged with the increase of AS. The relative deviation for most of the present calculated transition probabilities from different gauges is <10%. The good convergence properties of the E2 transition wavelength and probabilities and the agreement of calculated E2 transition probabilities in different gauges indicate the accuracy of the wavefunction to some extent. Most values of the transition wavelengths and probabilities agree well with the theoretical results by RMBPT [7]. The difference between our work and the work from RMBPT [7] is mainly due to the correlation effects for 3s and 3p orbitals which were omitted in the latter. The detailed contribution from the correlation of 3s and 3p orbitals will be discussed in another paper [19].

3.2. E1 transitions between [Ne]3s23p53d4–[Ne]3s23p3d2 configurations

The first excited state configuration of the W54+ ion is [Ne]3s23p53d4, with open p and d orbitals. It should be noted that

\[ \text{number of configurations for excited states ([Ne]3s}^23p^53d^4) \text{ in the 6SD(6s–6d) model is 1 651 545. It was found that an MCDF procedure for such a large scale ASF was not practically tractable with our present calculation resources. However, we found that both the energies and probabilities of M1 and E2 transitions between the ground state multiplets were almost convergent up to the calculations in the 5SD(5s–5d) and 5SD correlation models. We have assumed that the same also holds for the singly excited [Ne]3s}^23p^3d^4 configurations. Thus, we have performed the active space procedure in MCDF calculations up to the 5SD(5s–5d) correlation models for both the ground and excited state configurations.

Some E1 transition wavelengths λ (in nm) and probabilities A (in s−1) in the Coulomb (C) and Babushkin (B) gauges from [Ne]3s23p5d4 to [Ne]3s23p3d2 in different correlation models are listed in tables 6 and 7, respectively. It can be seen from these two tables that the quality of the convergence of the transition wavelengths and A-values is good. The final E1
transition wavelengths $\lambda$ (in nm), probabilities $A$ (in s\(^{-1}\)) and oscillator strengths $g_f$ are presented in table 8. The experimental observation by EBIT [11] and theoretical values from Flexible Atomic Code (FAC) [11] and MCDF [12] are also included in table 8 for comparison. The $j\,l$ coupling labels were adopted for the main component. For the transition energies ($E$), the results are in excellent agreement with the experimental data except for the first transition, i.e. $[(3p_1^3j/2\,3p_3^1j/2)_{3/2}(3d_2^0j/2)_{3/2}]_2 \rightarrow [3p^53d_{3/2}]_2$. According to the experiment, this observed line is affected by a blend with another Ti-like tungsten transition and this explains the significant difference between our calculated wavelength and the measurement. Comparing with the FAC results from Lennartsson et al [11], our calculation values are generally smaller than their data and all are in better agreement with the experimental data. They measured the wavelengths of 3p–3p and 3p–3d transitions in Al through Co-like W ions and calculated the corresponding atomic structures and line intensities using FAC. The configuration with singly excited L-shell electrons in addition to singly and also several multiply excited M-shell electron configurations were included in the calculation. For one of the early calculations by Dipti et al [12], we find substantial differences from the present calculations in both the values of transition energies and oscillator strengths. The origin of this difference may be interpreted as due to the difference in the size of the correlation space; we have adopted an active space method and the effect of the electron correlations systematically up to the convergence. For the transition probabilities ($A$) of the present calculation, all the relative deviations in Babushkin and Coulomb gauges are <10%. Only the results in Babushkin gauge are given in table 8.

It should be pointed out that about 466 E1 transitions could possibly be found from $3p^33p^3$ to $3p^53d^2$. In the present work, only the results having large transition probabilities ($>10^{12}$ s\(^{-1}\)) and the results having corresponding experimental data are listed in table 8. According to the present calculation, it was found that the transition energies could be divided by energy into two groups in about 2.95–3.25 nm and 1.86–1.96 nm. The previous EBIT measurements [11] were carried out in the wavelength range of 26.5–43.5 Å. According to the present calculation, it is suggested to make a new observation in the 1.86–1.96 nm wavelength range to look for the strong transitions predicted by the present work.
Table 8. Transition wavelength $\lambda$ (in nm) and radiative strengths $A$ (in s$^{-1}$) and the oscillator strengths (gf) in the Babushkin (B) gauge for E1 transitions in a Ca-like tungsten ion. Notation (a) for $A$ and (gf) means $a \times 10^6$.

| Lower | Upper | $\lambda_{\text{Present}}$ | $\lambda_{\text{Exp}}$ | Other | $A_{\text{Present}}$ | $A_{\text{Other}}$ |
|-------|-------|---------------------------|---------------------|-------|-------------------|------------------|
| $[3p^63d_{5/2}l_2]$ | $[(3p_{l/2}^3 3p_{l/2}^3)_{1/2}3d_{5/2}(3d_{5/2})_h]_{3/2}3d_{5/2}$ | 3.2401 | 3.2264 | 3.2416 | 8.500(10) | 6.69(2) | 6.85(2) |
| $[3p^63d_{5/2}l_2]$ | $[(3p_{l/2}^3 3p_{l/2}^3)_{1/2}3d_{5/2}(3d_{5/2})_h]_{3/2}3d_{5/2}$ | 3.1787 | 3.1811 | 3.1786 | 7.443(11) | 3.38(1) | 2.34(1) |
| $[3p^63d_{5/2}l_2]$ | $[(3p_{l/2}^3 3p_{l/2}^3)_{1/2}3d_{5/2}(3d_{5/2})_h]_{3/2}3d_{5/2}$ | 3.1732 | 3.1776 | 3.171 | 5.911(11) | 6.25(1) | 4.89(1) |
| $[3p^63d_{5/2}l_2]$ | $[(3p_{l/2}^3 3p_{l/2}^3)_{1/2}3d_{5/2}(3d_{5/2})_h]_{3/2}3d_{5/2}$ | 3.1536 | 3.1563 | 3.1505 | 9.425(11) | 7.03(1) | 8.31(1) |
| $[3p^63d_{5/2}l_2]$ | $[(3p_{l/2}^3 3p_{l/2}^3)_{1/2}3d_{5/2}(3d_{5/2})_h]_{3/2}3d_{5/2}$ | 3.1410 | 3.1430 | 3.1386 | 5.184(11) | 5.37(1) | 1.52(0) |
| $[3p^63d_{5/2}l_2]$ | $[(3p_{l/2}^3 3p_{l/2}^3)_{1/2}3d_{5/2}(3d_{5/2})_h]_{3/2}3d_{5/2}$ | 3.1251 | 3.1245 | 3.1155 | 9.331(11) | 4.10(1) | 4.37(1) |
| $[3p^63d_{5/2}l_2]$ | $[(3p_{l/2}^3 3p_{l/2}^3)_{1/2}3d_{5/2}(3d_{5/2})_h]_{3/2}3d_{5/2}$ | 3.1115 | 3.1157 | 3.1155 | 1.017(12) | 1.68(1) | 1.17(0) |
| $[3p^63d_{5/2}l_2]$ | $[(3p_{l/2}^3 3p_{l/2}^3)_{1/2}3d_{5/2}(3d_{5/2})_h]_{3/2}3d_{5/2}$ | 3.0947 | 3.1162 | 3.1162 | 3.0898 | 1.16(12) | 1.16(0) |
| $[3p^63d_{5/2}l_2]$ | $[(3p_{l/2}^3 3p_{l/2}^3)_{1/2}3d_{5/2}(3d_{5/2})_h]_{3/2}3d_{5/2}$ | 2.9530 | 2.9560 | 2.9452 | 2.9588(12) | 1.16(1) | 6.66(2) |
| $[3p^63d_{5/2}l_2]$ | $[(3p_{l/2}^3 3p_{l/2}^3)_{1/2}3d_{5/2}(3d_{5/2})_h]_{3/2}3d_{5/2}$ | 1.9603 | 1.9620 | 1.9620 | 1.9163 | 1.926(12) | 7.42(1) |
| $[3p^63d_{5/2}l_2]$ | $[(3p_{l/2}^3 3p_{l/2}^3)_{1/2}3d_{5/2}(3d_{5/2})_h]_{3/2}3d_{5/2}$ | 1.9340 | 1.9340 | 1.9340 | 1.9084 | 1.947(12) | 5.53(1) |
| $[3p^63d_{5/2}l_2]$ | $[(3p_{l/2}^3 3p_{l/2}^3)_{1/2}3d_{5/2}(3d_{5/2})_h]_{3/2}3d_{5/2}$ | 1.9266 | 1.9266 | 1.9266 | 1.9078 | 3.003(12) | 8.19(1) |
| $[3p^63d_{5/2}l_2]$ | $[(3p_{l/2}^3 3p_{l/2}^3)_{1/2}3d_{5/2}(3d_{5/2})_h]_{3/2}3d_{5/2}$ | 1.9084 | 1.9084 | 1.9084 | 1.9060 | 2.597(12) | 7.07(1) |
| $[3p^63d_{5/2}l_2]$ | $[(3p_{l/2}^3 3p_{l/2}^3)_{1/2}3d_{5/2}(3d_{5/2})_h]_{3/2}3d_{5/2}$ | 1.8990 | 1.8990 | 1.8990 | 1.8970(12) | 1.07(0) |
| $[3p^63d_{5/2}l_2]$ | $[(3p_{l/2}^3 3p_{l/2}^3)_{1/2}3d_{5/2}(3d_{5/2})_h]_{3/2}3d_{5/2}$ | 1.8865 | 1.8865 | 1.8865 | 1.8861 | 1.956(12) | 7.30(1) |
| $[3p^63d_{5/2}l_2]$ | $[(3p_{l/2}^3 3p_{l/2}^3)_{1/2}3d_{5/2}(3d_{5/2})_h]_{3/2}3d_{5/2}$ | 1.8852 | 1.8852 | 1.8852 | 1.8852 | 2.148(12) | 8.01(1) |
| $[3p^63d_{5/2}l_2]$ | $[(3p_{l/2}^3 3p_{l/2}^3)_{1/2}3d_{5/2}(3d_{5/2})_h]_{3/2}3d_{5/2}$ | 4.483(12) | 4.483(12) | 4.483(12) | 1.8852 | 4.483(12) | 7.17(1) |
| $[3p^63d_{5/2}l_2]$ | $[(3p_{l/2}^3 3p_{l/2}^3)_{1/2}3d_{5/2}(3d_{5/2})_h]_{3/2}3d_{5/2}$ | 8.059(12) | 8.059(12) | 8.059(12) | 1.8593 | 5.089(12) | 7.91(1) |

\[a\] This work.
\[b\] From Lennartsson by EBIT and the collisional-radiative model [11].
\[c\] From Dipti et al. by the MCDF method [12].

For the transitions in 2.95–3.25 nm, it is found that most observed transitions have large transition probabilities. However, a few transitions in this range with large transition probabilities have not been observed in the previous EBIT experiment [11]. This might be because the population of the excited upper levels of these unobserved transitions is small. A collisional-radiative model analysis on the transition intensities within the EBIT experiment had been performed for the W$^{26+}$ ion [20]. A similar model was applied to investigate the population of the excited states and the intensity of the transitions of the W$^{54+}$ ion. The results show that the intensities of the transition lines which could not be observed are generally smaller by four orders of magnitude than the intensities which could be observed. The intensity changes with the plasma conditions. It is suggested that these transition lines could be observed by some appropriate plasma conditions.
In addition, it must be pointed out that the Ca-I (3.1430 nm) and Ca-6 (3.1776 nm) in the experiment [11, 12] have the same label for the state designation. This is due to the convention to use a leading configuration in ASF for the state assignment. According to the present calculation, the CSF components of the upper level of the transition with wavelength 3.1430 nm are 45.36% from $[(3p^{2}J_{1/2})^{2}(3d^{2}J_{5/2})_{h}j_{2}3d_{5/2}]_{J_{3}3}$, 29.13% from $[(3p^{2}J_{1/2})^{2}(3d^{2}J_{5/2})_{h}j_{2}3d_{5/2}]_{J_{3}3}$, $13.60\%$ from $[(3p^{2}J_{1/2})^{2}(3d^{2}J_{5/2})_{h}j_{2}3d_{5/2}]_{J_{3}3}$, and $4.34\%$ from $[(3p^{2}J_{1/2})^{2}(3d^{2}J_{5/2})_{h}j_{2}3d_{5/2}]_{J_{3}3}$, whereas the CSF components of the upper level of the transition with wavelength 3.1776 nm are 35.63% from $[(3p^{2}J_{1/2})^{2}(3d^{2}J_{5/2})_{h}j_{2}3d_{5/2}]_{J_{3}3}$, $20.77\%$ from $[(3p^{2}J_{1/2})^{2}(3d^{2}J_{5/2})_{h}j_{2}3d_{5/2}]_{J_{3}3}$, $17.47\%$ from $[(3p^{2}J_{1/2})^{2}(3d^{2}J_{5/2})_{h}j_{2}3d_{5/2}]_{J_{3}3}$, $13.53\%$ from $[(3p^{2}J_{1/2})^{2}(3d^{2}J_{5/2})_{h}j_{2}3d_{5/2}]_{J_{3}3}$ and $5.08\%$ from $[(3p^{2}J_{1/2})^{2}(3d^{2}J_{5/2})_{h}j_{2}3d_{5/2}]_{J_{3}3}$. It is suggested to indicate the second leading terms to discriminate the states in such a case.

4. Conclusions

The E1, M1, E2 transition energies and probabilities were calculated by the MCDF method with electron correlation effects taken into account systematically and efficiently. A reliable correlation model is offered on the basis of doing a great number of calculations. In addition, some important correlation effects are pointed out compared with previous work. Finally, several strong E1 transitions were predicted that might be observed in future experiments.

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