# Study On Electron Collisions With Zn-like W Ion

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**Abstract.** The present work gives new refined results for electron impact excitation rates and collision strengths for transitions of type $[Ar]3d^{10}4snl$–>$[Ar]3d^{10}4sn'l'$, $n, n'$=4,5, and $\Delta J$=0,1in Zn-like W ion. We have examined the position and widths of the resonant states of type $1s^2 2s 2p^6 3s^2 3p^6 3d^{10} 4s^2 nl$. Autoionizing states can radically alter the low temperature behavior of collision rates, and are a major contributor to opacity. Preliminary results for Auger rates are presented. Hartree-Fock calculations have been carried out followed by a configuration interaction (CI) in intermediate coupling using the suite of Cowan's codes.

**Keywords:** Zn-like W ion, atomic structure calculation, collision data, Auger rates.
**PACS:** 31.15.xr, 32.80.Hd, 32.80.Zb, 31.15.xp, 52.20.Fs, 52.25.Vy.

## INTRODUCTION

The radiation emission and spatial distribution of high Z-materials will influence plasma performance for ITER. At one level, the interpretation of spectra from fusion plasmas requires knowledge of the processes that populate atomic and molecular energy levels that give rise to emission and absorption. But at a more fundamental level, the construction of predictive models requires secure knowledge of the basic atomic processes in the plasma. Atomic structure calculation for $W^{44+}$ has been reported [1, 2]. Technological development of powerful lasers and fusion devices such as tokamaks has triggered a significant progress in what concerns spectroscopic investigations of structure of highly ionized atoms. Line spectra examination of such ions is one of the methods employed for plasma parameters diagnostics. The 4s – 4p, 4p – 4d, and 4d – 4f transitions of ten copper-like and zinc-like ions from $Ba^{26+}$ to $W^{45+}$ have been observed by means of a laser-produced plasmas[1] and the results supported the identification of the resonance lines of $Xe^{24+}$ and $Xe^{25+}$ in the Princeton University ST tokamak[2]. As tokamak systems become increasingly more sophisticated, the ability to predict and monitor plasma properties becomes imperative. The radiation emission and spatial distribution of high Z-materials penetrates the core plasma, tungsten exhibiting high specific radiation losses. Consequently, a significant fraction of the energy may be exhausted via the radiation emitted by these ions and this leads to plasma cooling. It is important, then, to have accurate data on which to base these predictions.

A study of tungsten impurity spectrum at the ASDEX Upgrade tokamak[3] reported that for electron temperature above 2keV, many isolated spectral lines appear in the spectrum which superimposed the quasi-continuum emission band. These lines represent transitions in the highly charged tungsten ions (up to Cu-like $W^{45+}$) and were identified by means of wavelengths predicted using the HULLAC package [4]. Atomic data for tungsten and for a series of other ions with Z ranging between 60 and 92 have been given by Zang et al.[5] and wavelengths and line intensities in tungsten have been calculated by Fournier[6]. The production of high quality atomic data for X-ray spectroscopy is rather complicated as the high energy conditions of the emitting plasmas demand the study of large numbers of energy levels as well as inner-shell and Auger processes.

Atomic structure calculation for $W^{44+}$ has previously been reported [7, 8].This work provides new refined results for electron impact excitation rates and collision strengths for transitions of type $[Ar]3d^{10}4snl$ –>$[Ar]3d^{10}4sn'l'$, $n,n'$=4,5, and $\Delta J$=0,1. The modeling is based on the Hartree-Fock formalism and collision data are obtained by means of plane-wave Born method. Also presented are preliminary results for Auger rates. We have examined the positions and widths of resonant states of type $1s^2 2s 2p^6 3s^2 3p^6 3d^{10} 4s^2 nl$.

## MODELING AND RESULTS

In order to compute atomic structure of ions, we used the atomic structure code of Cowan [9] that uses the superposition-of-configuration method. This code has also been widely employed by many researchers [10] who computed energy levels and oscillator strengths for many ions of astrophysical interest. In order to increase accuracy of calculation, the *jj*-coupling scheme and relativistic effects have been included. In case of heavy ions such as tungsten ones, relativistic effects are important even for allowed transitions. The corrections applied to total binding energies are quite large and the main contribution comes from the tightly bound inner electrons. Therefore, it is sufficient to calculate the Darwin and the mass-velocity corrections as a relativistic correction to the total binding energy. When calculating excitation and ionization energies, the correlation energy becomes highly important. This can be calculated with the aid of theoretical results on correlation energy of a free-electron gas- approach already applied by many authors [11, 12] to Thomas-Fermi as well as to self-consistent field calculations. Unfortunately, these corrections still prove to be too large and this is due to the fact that there are differences between the free electron gas and the tightly bound electrons in the atom.

The first part of this work presents new collision data for transitions of type $[Ar]3d^{10}\ 4s\ nl$ -> $[Ar]3d^{10}\ 4s\ n'l'$ with $n,n'$=4,5 and $l,l'$=0,1,2,3, for $\Delta J$=0,1 in the Zn-like isoelectronic sequences of tungsten. The configurations that have been studied are tagged as follows: **1**-$[Ar]\ 3d^{10}4s^2$, **2**-$[Ar]\ 3d^{10}\ 4s\ 4p$, **3**-$[Ar]\ 3d^{10}\ 4s\ 4d$, **4**-$[Ar]\ 3d^{10}\ 4s\ 4f$, **5**-$[Ar]\ 3d^{10}\ 4s\ 5s$, **6**-$[Ar]\ 3d^{10}\ 4s\ 5p$, **7**-$[Ar]\ 3d^{10}\ 4s\ 5d$, **8**-$[Ar]\ 3d^{10}\ 4s\ 5f$. In order to calculate collision strengths- in case of excitation by electron impact processes- the code uses the plane wave Born method. This approximation has certain drawbacks. For instance, since plane waves are employed, this method does not account for the electron exchange effect with the target electrons. Also disregarded, are the distortion

of the plane wave in the vicinity of the Zn-like ion target and the polarization of the target due to the presence of the incident electron. Hence, PWB is strictly applicable – with accurate results- at high energies and for spin-allowed transitions. However, the interdiction for spin-forbidden transitions is valid only for pure *LS*-coupling scheme.

The total collision strengths are obtained from electron-impact excitation cross-sections according to the formula:

$$\Omega_{JJ'}(\varepsilon) = \varepsilon \cdot g \cdot Q_{JJ'}(\varepsilon) = \frac{8}{\Delta E} \cdot \int_{K\,\min}^{K\,\max} g f_{JJ'}(K) d(\ln K) \qquad (1)$$

$\Omega_{JJ'}(\varepsilon)$ is the total collision strength, *J* and *J'* denoting the quantum numbers of the respective levels. $Q_{JJ'}$ represents the total cross-section, $\Delta E$ is the excitation energy that enables the transition $J \to J'$, $\varepsilon = k^2 \geq \Delta E$ is the kinetic energy of the impacting electron, $g = 2J + 1$ the statistical weight of the $J$ level and $f_{JJ'}(K)$ is the generalized oscillator strength. Results are presented in Table 1.

**TABLE 1**. Total collision strengths. For each transition Tr., and at temperature T (units of eV), the corresponding collision strength is given. $5.1588^{-01}$ reads as $5.1588 \times 10^{-1}$.

| Tr. | T=500 (eV) | T=700 (eV) | T=1000 (eV) | T=1500 (eV) | T=2000 (eV) | T=3000 (eV) | T=5000 (eV) |
|---|---|---|---|---|---|---|---|
| 7-8 | $19.5674^{00}$ | $20.5149^{00}$ | $21.4820^{00}$ | $22.4644^{00}$ | $23.4572^{00}$ | $24.4575^{00}$ | $25.4638^{00}$ |
| 5-6 | $7.0680^{00}$ | $7.3977^{00}$ | $7.7341^{00}$ | $8.0752^{00}$ | $8.4202^{00}$ | $8.7680^{00}$ | $9.1176^{00}$ |
| 3-2 | $5.0731^{00}$ | $5.3081^{00}$ | $5.5478^{00}$ | $5.7911^{00}$ | $6.0372^{00}$ | $6.2849^{00}$ | $6.5340^{00}$ |
| 1-2 | $1.3623^{00}$ | $1.4220^{00}$ | $1.4829^{00}$ | $1.5447^{00}$ | $1.6071^{00}$ | $1.6700^{00}$ | $1.7332^{00}$ |
| 4-8 | $5.2501^{-01}$ | $5.3321^{-01}$ | $5.4055^{-01}$ | $5.4713^{-01}$ | $5.5296^{-01}$ | $5.5799^{-01}$ | $5.6251^{-01}$ |
| 3-7 | $3.7928^{-01}$ | $3.8683^{-01}$ | $3.9354^{-01}$ | $3.9950^{-01}$ | $4.0477^{-01}$ | $4.0938^{-01}$ | $4.1344^{-01}$ |
| 2-6 | $2.0111^{-01}$ | $2.0564^{-01}$ | $2.0969^{-01}$ | $2.1327^{-01}$ | $2.1642^{-01}$ | $2.1917^{-01}$ | $2.2159^{-01}$ |
| 7-4 | $1.1147^{-01}$ | $1.2188^{-01}$ | $1.3289^{-01}$ | $1.4458^{-01}$ | $1.5676^{-01}$ | $1.6932^{-01}$ | $1.8217^{-01}$ |
| 7-2 | $1.0336^{-01}$ | $1.1744^{-01}$ | $1.3256^{-01}$ | $1.4861^{-01}$ | $1.6549^{-01}$ | $1.8307^{-01}$ | $2.0130^{-01}$ |
| 5-2 | $8.4117^{-02}$ | $9.4292^{-02}$ | $1.0508^{-01}$ | $1.1638^{-01}$ | $1.2814^{-01}$ | $1.4031^{-01}$ | $1.5282^{-01}$ |
| 1-5 | $3.1117^{-02}$ | $3.1836^{-02}$ | $3.2485^{-02}$ | $3.3059^{-02}$ | $3.3563^{-02}$ | $3.4010^{-02}$ | $3.4409^{-02}$ |
| 1-6 | $1.5280^{-02}$ | $1.6969^{-02}$ | $1.8807^{-02}$ | $2.0775^{-02}$ | $2.2879^{-02}$ | $2.5093^{-02}$ | $2.7395^{-02}$ |
| 6-6 | $1.093^{-06}$ | $1.096^{-06}$ | $1.098^{-06}$ | $1.099^{-06}$ | $1.099^{-06}$ | $1.100^{-06}$ | $1.100^{-06}$ |
| 7-7 | $2.71^{-07}$ | $2.91^{-07}$ | $3.10^{-07}$ | $3.28^{-07}$ | $3.44^{-07}$ | $3.57^{-07}$ | $3.68^{-07}$ |

Excitation rate coefficients have been calculated from the total collision strengths by integration over a Maxwellian distribution for temperatures ranging between 1 and 2000 eV for low excitation energies and temperatures between 5 and 10000 eV for high excitation energies (for highly ionized atoms). Results are given in Table 2.

The second part of our work concerns continuum simulations involving autoionization probabilities in case of Auger effect. For this purpose, bound-continuum configuration-interaction matrix elements are calculated and the values of the Auger rates are computed by means of first-order perturbation theory according to equation (2).

$$A_{ji}^{a} = \frac{2\pi}{\hbar} |\langle jHi \rangle|^2 = \frac{2\pi}{\hbar} |\sum_{bb'} \langle j|b\rangle \langle b|H|b'\rangle \langle b'|i\rangle|^2 \qquad (2)$$

**TABLE 2**. Excitation rate coefficients ($cm^3s^{-1}$). For each transition Tr., at temperature T (units of eV) the excitation rate coefficient is given (units of $cm^3s^{-1}$). $1.3626^{-09}$ reads as $1.3626\times10^{-9}$.

| Tr. | T=500 (eV) | T=700 (eV) | T=1000 (eV) | T=1500 (eV) | T=2000 (eV) | T=3000 (eV) | T=5000 (eV) |
|---|---|---|---|---|---|---|---|
| 7-8 | $1.3101^{-09}$ | $1.2506^{-09}$ | $1.1750^{-09}$ | $1.0803^{-09}$ | $1.0107^{-09}$ | $9.1230^{-10}$ | $7.9235^{-10}$ |
| 5-6 | $4.7211^{-10}$ | $4.4957^{-10}$ | $4.2132^{-10}$ | $3.8633^{-10}$ | $3.6079^{-10}$ | $3.2495^{-10}$ | $2.8154^{-10}$ |
| 3-2 | $2.2197^{-10}$ | $2.2368^{-10}$ | $2.1906^{-10}$ | $2.0853^{-10}$ | $1.9892^{-10}$ | $1.8367^{-10}$ | $1.6323^{-10}$ |
| 1-2 | $6.5369^{-11}$ | $6.4768^{-11}$ | $6.2550^{-11}$ | $5.8795^{-11}$ | $5.5665^{-11}$ | $5.0928^{-11}$ | $4.4823^{-11}$ |
| 4-8 | $7.5199^{-12}$ | $9.4641^{-12}$ | $1.0776^{-11}$ | $1.1316^{-11}$ | $1.1199^{-11}$ | $1.0550^{-11}$ | $9.2827^{-12}$ |
| 3-7 | $7.9953^{-12}$ | $1.0677^{-11}$ | $1.2739^{-11}$ | $1.3917^{-11}$ | $1.4081^{-11}$ | $1.3602^{-11}$ | $1.2261^{-11}$ |
| 7-4 | $1.4905^{-12}$ | $1.8762^{-12}$ | $2.2053^{-12}$ | $2.4860^{-12}$ | $2.6358^{-12}$ | $2.7887^{-12}$ | $2.8922^{-12}$ |
| 2-6 | $1.7375^{-12}$ | $2.4681^{-12}$ | $3.0874^{-12}$ | $3.5062^{-12}$ | $3.6219^{-12}$ | $3.5799^{-12}$ | $3.2972^{-12}$ |
| 5-2 | $5.1378^{-13}$ | $7.4354^{-13}$ | $9.8492^{-13}$ | $1.2435^{-12}$ | $1.4139^{-12}$ | $1.6316^{-12}$ | $1.8544^{-12}$ |
| 1-5 | $4.2532^{-13}$ | $6.3322^{-13}$ | $8.2054^{-13}$ | $9.5804^{-13}$ | $1.0039^{-12}$ | $1.0074^{-12}$ | $9.4048^{-13}$ |
| 7-2 | $4.0828^{-13}$ | $6.4240^{-13}$ | $9.0329^{-13}$ | $1.1970^{-12}$ | $1.4014^{-12}$ | $1.6823^{-12}$ | $2.0089^{-12}$ |
| 1-6 | $8.1095^{-14}$ | $1.2683^{-13}$ | $1.7263^{-13}$ | $2.1517^{-13}$ | $2.3918^{-13}$ | $2.6683^{-13}$ | $2.9496^{-13}$ |
| 6-6 | $6.3159^{-17}$ | $5.5344^{-17}$ | $4.7613^{-17}$ | $3.9760^{-17}$ | $3.4840^{-17}$ | $2.8802^{-17}$ | $2.2555^{-17}$ |
| 7-7 | $4.6358^{-17}$ | $4.1248^{-17}$ | $3.6228^{-17}$ | $3.1086^{-17}$ | $2.7811^{-17}$ | $2.3701^{-17}$ | $1.9301^{-17}$ |
| 2-2 | $4.6502^{-17}$ | $4.2185^{-17}$ | $3.7269^{-17}$ | $3.1794^{-17}$ | $2.8170^{-17}$ | $2.3562^{-17}$ | $1.8642^{-17}$ |

**TABLE 3.** Auger rates. For each level, the Auger rate is given in units of $sec^{-1}$. $5.115^{+13}$ reads as $5.115\times10^{-13}$.

| Configuration type $1s^2\ 2s\ 2p^5\ 3s^2\ 3d^{10}\ 4s^2\ nl$ | J | Auger rate (units of $sec^{-1}$) | Configuration type $1s^2\ 2s\ 2p^5\ 3s^2\ 3d^{10}\ 4s^2 nl$ | J | Auger rate (units of $sec^{-1}$) |
|---|---|---|---|---|---|
| [Ar] 2s $4s^2$ 5p | 1 | $5.115^{+13}$ | [Ar] 2s $4s^2$ 10p | 1 | $4.38577^{+12}$ |
| [Ar] 2s $4s^2$ 5p | 1 | $2.457^{+13}$ | [Ar] 2s $4s^2$ 7p | 1 | $4.3^{+12}$ |
| [Ar] 2s $4s^2$ 5p | 0 | $2.312^{+13}$ | [Ar] 2s $4s^2$ 8p | 0 | $4.17935^{+12}$ |
| [Ar] 2s $4s^2$ 5p | 2 | $2.312^{+13}$ | [Ar] 2s $4s^2$ 8p | 2 | $4.17935^{+12}$ |
| [Ar] 2s $4s^2$ 5s | 1 | $1.788^{+13}$ | [Ar] 2s $4s^2$ 7d | 2 | $4.05066^{+12}$ |
| [Ar] 2s $4s^2$ 5d | 1 | $1.749^{+13}$ | [Ar] 2s $4s^2$ 8d | 1 | $3.91207^{+12}$ |
| [Ar] 2s $4s^2$ 5d | 3 | $1.749^{+13}$ | [Ar] 2s $4s^2$ 8d | 3 | $3.91207^{+12}$ |
| [Ar] 2s $4s^2$ 5p | 1 | $1.562^{+13}$ | [Ar] 2s $4s^2$ 8s | 1 | $3.71341^{+12}$ |
| [Ar] 2s $4s^2$ 7p | 1 | $1.549^{+13}$ | [Ar] 2s $4s^2$ 6p | 1 | $3.4532^{+12}$ |
| [Ar] 2s $4s^2$ 5s | 0 | $1.341^{+13}$ | [Ar] 2s $4s^2$ 7s | 0 | $3.43859^{+12}$ |
| [Ar] 2s $4s^2$ 5d | 2 | $1.196^{+13}$ | [Ar] 2s $4s^2$ 6d | 2 | $3.08978^{+12}$ |
| [Ar] 2s $4s^2$ 6p | 0 | $1.064^{+13}$ | [Ar] 2s $4s^2$ 9p | 0 | $2.86764^{+12}$ |
| [Ar] 2s $4s^2$ 6p | 2 | $1.064^{+13}$ | [Ar] 2s $4s^2$ 9p | 2 | $2.86764^{+12}$ |
| [Ar] 2s $4s^2$ 6d | 1 | $9.70843^{+12}$ | [Ar] 2s $4s^2$ 8p | 1 | $2.82155^{+12}$ |
| [Ar] 2s $4s^2$ 6d | 3 | $9.70843^{+12}$ | [Ar] 2s $4s^2$ 9d | 1 | $2.71501^{+12}$ |
| [Ar] 2s $4s^2$ 6s | 1 | $9.61162^{+12}$ | [Ar] 2s $4s^2$ 9d | 3 | $2.71501^{+12}$ |
| [Ar] 2s $4s^2$ 5p | 1 | $7.5^{+12}$ | [Ar] 2s $4s^2$ 8d | 2 | $2.65849^{+12}$ |
| [Ar] 2s $4s^2$ 7p | 1 | $7.45^{+12}$ | [Ar] 2s $4s^2$ 9s | 1 | $2.53669^{+12}$ |
| [Ar] 2s $4s^2$ 6p | 1 | $7.18218^{+12}$ | [Ar] 2s $4s^2$ 6p | 1 | $2.18802^{+12}$ |
| [Ar] 2s $4s^2$ 6d | 2 | $6.61865^{+12}$ | [Ar] 2s $4s^2$ 8s | 0 | $2.11891^{+12}$ |
| [Ar] 2s $4s^2$ 7p | 0 | $6.3707^{+12}$ | [Ar] 2s $4s^2$ 10p | 1 | $2.11134^{+12}$ |
| [Ar] 2s $4s^2$ 7p | 2 | $6.3707^{+12}$ | [Ar] 2s $4s^2$ 7p | 1 | $2.07^{+12}$ |
| [Ar] 2s $4s^2$ 6s | 0 | $6.25072^{+12}$ | [Ar] 2s $4s^2$ 10d | 1 | $1.95302^{+12}$ |
| [Ar] 2s $4s^2$ 7d | 1 | $5.95323^{+12}$ | [Ar] 2s $4s^2$ 10d | 3 | $1.95302^{+12}$ |
| [Ar] 2s $4s^2$ 7d | 3 | $5.95323^{+12}$ | [Ar] 2s $4s^2$ 9p | 1 | $1.93585^{+12}$ |
| [Ar] 2s $4s^2$ 7s | 1 | $5.74234^{+12}$ | [Ar] 2s $4s^2$ 7d | 2 | $1.90257^{+12}$ |
| [Ar] 2s $4s^2$ 5d | 2 | $5.53^{+12}$ | [Ar] 2s 4s2 9d | 2 | $1.84348^{+12}$ |

The intermediate- coupling eigenvector components $\langle j|b\rangle$ for the pure-discrete (but potentially autoionizing) state j and the components $\langle b'|i\rangle$ for the pure continuum state i are obtained from the energy-matrix diagonalization. The investigated resonant states were of type $1s^2 2s 2p^6 3s^2 3p^6 3d^{10} 4s^2 nl$, with n=4,5,6,7,8,9,10 and $l$=0,1,2,3.

The hypothesis used was that the Auger effect occurs as an indirect phenomenon. An inner subshell electron is excited into a high state via dielectronic capture of the impacting electron. This is followed by autoionization by Auger Effect into a state of the target atom different from the original one.

## CONCLUSIONS

This paper presents collision data and Auger rates for Zn-like W ion. Using the atomic structure code of Cowan, and through the Hartree-Fock approximation, we have calculated collision strengths and excitation rate coefficients in the plane wave-Born approximation. Neglected phenomena that are disregarded due to the employment of plane waves, are not of any concern in case of simulations involving high energies, spin-allowed transitions or calculations in *jj*-coupling scheme for spin-forbidden transitions.

This paper also presents a series of autoionization probabilities in case of indirect Auger effect for states of type $1s^2\ 2s\ 2p^5\ 3s^2\ 3d^{10}\ 4s^2\ nl$.

In order to fully characterize the complex behavior of Zn-like tungsten ions, further simulations are necessary, implying more excited configurations, continuum calculations and different approximations for modeling atomic structure.

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