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Atomic Data For Zn-like W Ion As Related To The Plasma Modelling

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1. INTRODUCTION

Energetic, hot plasmas can be produced by various means from controlled fusion experiments based on tokamak discharges to high-power laser irradiation of solid, or, as it has also been proposed, by intense ion beam striking a fuel pellet.

To analyze the plasma conditions reached, one has to identify characteristic spectral lines that reveal the presence of specific highly charged ions, to evaluate relative line intensities or to measure line widths for deriving an ion temperature. Furthermore, for a proper interpretation of the spectra of these species, it is compulsory to develop a theoretical modelling in order to expand the limited experimental spectral data.

This work's aim is to report atomic data for tungsten ions belonging to Zn-like isoelectronic sequences.

2. CALCULATIONS AND COMPUTATIONAL IMPLEMENTATIONS

Due to the high temperature in the plasma, the tungsten ions reach high ionization stages and the radiation of the element occurs mainly in the far ultraviolet (VUV), extreme ultraviolet (EUV) and X ray regions. There have been many measurements of particular lines and many theoretical predictions of transitions. Atomic data for tungsten (and for a series of other ions with Z ranging between 60 and 92) have been given by Zhang et al.[2] whereas Aggarwal et al.[3] have provided data for modeling of lasers for W XXXXVII and various Ni-like ions. However, the most complete compilations of the wavelengths and intensities of lines in tungsten belong to Fournier [4].

This work presents collision data for transitions of type $[Ar]3d^{10}\,4s\,nl \rightarrow [Ar]4s\,n'l'$ with $n, n' = 4, 5$ and $l, l' = 0, 1, 2, 3$, for $\Delta J = 0, 1$. The configurations that have been used 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**- $[Ar]\,3d^{10}\,4s\,5f$. The atomic structure code of Cowan was used to output the plane-wave-Born collision strengths. This suite of four programs calculates atomic structures and spectra via superposition-of-configuration method.

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The radial wavefunctions are calculated, through the Hartree-Fock method, for each of any number of the specified configurations. Furthermore, the higher orbitals that have been included and the large number of configurations improves the quality of these wavefunctions, wavefunctions that are used to compute the Coulomb integrals and the spin-orbit integrals, along with the radial integrals required to give kinetic and electron-nuclear energies and rough relativistic and correlation corrections to both the one-electron binding energies and the total electronic binding energy. Using this information, the code further calculates configuration-interaction radial Coulomb integrals and the reduced matrix elements of spherical Bessel functions and scales all the energy-level-structure parameters. Next, come the energy matrices for each possible value of the total angular momentum J. Each matrix is diagonalized to get eigenvalues (energy levels) and eigenvectors. The electric dipole and quadrupole radiation spectra are computed, with wavelengths, oscillator strengths, radiative transition probabilities and radiative lifetimes.

It is worth mentioning that the calculations were performed in *jj*- coupling scheme. Together with the relativistic effects (included option) this ensures that the quantity of data is increased over the *LS*-coupled systems. These calculations involve a certain number of fine structure levels. The energy levels relative to the ground state [Ar]$3d^{10}4s^2$ are given in **Table 1**.

Table 1. **ENERGY LEVELS (units of 1000 cm^{-1})**

Config	State	Energy level	J	Config	State	Energy level	J
1	[Ar] $3d^{10}4s^2$	0	0				
2	[Ar] $3d^{10}4s\,4p$	6.6887^{02}	0	5	[Ar]$3d^{10}4s5s$	7.6870^{03}	0
2	[Ar] $3d^{10}4s\,4p$	7.2742^{02}	1	6	[Ar]$3d^{10}4s\,5p$	8.0215^{03}	0
2	[Ar] $3d^{10}4s\,4p$	1.5035^{03}	2	6	[Ar] $3d^{10}4s5p$	8.0286^{03}	1
2	[Ar] $3d^{10}4s\,4p$	1.6518^{03}	1	6	[Ar] $3d^{10}4s5p$	8.4109^{03}	2
3	[Ar] $3d^{10}4s4d$	2.7624^{03}	1	6	[Ar] $3d^{10}4s5p$	8.4258^{03}	1
3	[Ar] $3d^{10}4s4d$	2.7892^{03}	2	7	[Ar] $3d^{10}4s5d$	8.9875^{03}	1
3	[Ar] $3d^{10}4s4d$	2.9384^{03}	3	7	[Ar] $3d^{10}4s5d$	8.9916^{03}	2
3	[Ar] $3d^{10}4s4d$	3.0033^{03}	2	7	[Ar] $3d^{10}4s5d$	9.0721^{03}	3
4	[Ar] $3d^{10}4s\,4f$	4.2801^{03}	2	7	[Ar] $3d^{10}4s5d$	9.0792^{03}	2
4	[Ar] $3d^{10}4s\,4f$	4.2917^{03}	3	8	[Ar] $3d^{10}4s5f$	9.6612^{03}	2
4	[Ar] $3d^{10}4s\,4f$	4.3293^{03}	4	8	[Ar] $3d^{10}4s5f$	9.6639^{03}	3
4	[Ar] $3d^{10}4s\,4f$	4.3636^{03}	3	8	[Ar] $3d^{10}4s5f$	9.6870^{03}	4
5	[Ar] $3d^{10}4s5s$	7.6324^{03}	1	8	[Ar] $3d^{10}4s5f$	9.6918^{03}	3

As to what concerns the collision strengths data, the basic code output consists of the values of the momentum transfer and also for each spectrum line (or rather each *J-J'* excitation) the program provides values of the weighted generalized oscillator strength and those of the weighted transition probability *gA*. Also present, is a table containing values of x- the ratio between the kinetic energy of the impacting electron and the excitation energy- the kinetic energy, the unmodified collision strength Ω and also two modifications of Ω that should be physically more accurate at small x. Selected collision strengths are given below for different temperatures ranging from 500 to 3000 eV.

Table 2. TOTAL COLLISION STRENGTHS

Trans.	T=500(eV)	700(eV)	1000(eV)	1500(eV)	2000(eV)	3000(eV)
7-4	1.1147^{-01}	1.2189^{-01}	1.3290^{-01}	1.4458^{-01}	1.5676^{-01}	1.6932^{-01}
3-6	1.4418^{-01}	1.6041^{-01}	1.7758^{-01}	1.9559^{-01}	2.1428^{-01}	2.3354^{-01}
2-6	2.0115^{-01}	2.0568^{-01}	2.0973^{-01}	2.1331^{-01}	2.1645^{-01}	2.1921^{-01}
3-7	3.7936^{-01}	3.8690^{-01}	3.9362^{-01}	3.9958^{-01}	4.0485^{-01}	4.0946^{-01}
4-8	5.2510^{-01}	5.3330^{-01}	5.4064^{-01}	5.4722^{-01}	5.5305^{-01}	5.5808^{-01}
3-8	6.0714^{-01}	6.7833^{-01}	7.5324^{-01}	8.3140^{-01}	9.1221^{-01}	9.9522^{-01}
1-2	1.3627^{00}	1.4225^{00}	1.4834^{00}	1.5451^{00}	1.6075^{00}	1.67039^{00}
3-2	5.0728^{00}	5.3078^{00}	5.5475^{00}	5.7908^{00}	6.0368^{00}	6.2846^{00}
3-4	5.9981^{00}	6.2667^{00}	6.5405^{00}	6.8183^{00}	7.0988^{00}	7.3814^{00}
5-6	7.0660^{00}	7.3957^{00}	7.7319^{00}	8.0728^{00}	8.4177^{00}	8.7653^{00}
7-6	1.3474^{01}	1.4153^{01}	1.4846^{01}	1.5550^{01}	1.6263^{01}	1.6981^{01}
7-8	1.9557^{01}	2.0504^{01}	2.1471^{01}	2.2452^{01}	2.3444^{01}	2.4444^{01}

Accompanying the collision strengths are the excitation rate coefficients computed from the modified Ω by integration over Maxwellian distribution, at electron temperatures ranging from T_e=5 to 10000 eV and Table 3 presents a selection of these coefficients at different temperatures.

Collision data and the electric dipole and quadrupole transition probabilities are used to find the steady state collisional-radiative level populations in each ion. Once the collisional-radiative level populations are determined, line intensities can easily be obtained. Strong lines are radiated by tungsten ions isoelectronic to Zn because of their relatively simple electron configuration.

Table 3. EXCITATION RATE COEFFICIENTS (units of cm^3s^{-1})

Trans.	T=500(eV)	700(eV)	1000(eV)	1500(eV)	2000(eV)	3000(eV)
3-6	1.2840^{-12}	1.7326^{-12}	2.1718^{-12}	2.6129^{-12}	2.8880^{-12}	3.2191^{-12}
7-4	1.4907^{-12}	1.8765^{-12}	2.2056^{-12}	2.4863^{-12}	2.6360^{-12}	2.7889^{-12}
2-6	1.7380^{-12}	2.4687^{-12}	3.0882^{-12}	3.5070^{-12}	3.6227^{-12}	3.5807^{-12}
3-8	3.1504^{-12}	4.7189^{-12}	6.4201^{-12}	8.2757^{-12}	9.5030^{-12}	1.1060^{-11}
4-8	7.5217^{-12}	9.4662^{-12}	1.0778^{-11}	1.1318^{-11}	1.1201^{-11}	1.0552^{-11}
3-7	7.9974^{-12}	1.0680^{-11}	1.2742^{-11}	1.3921^{-11}	1.4084^{-11}	1.3605^{-11}
1-2	6.5434^{-11}	6.4825^{-11}	6.2598^{-11}	5.8835^{-11}	5.5700^{-11}	5.0957^{-11}
3-2	2.2196^{-10}	2.2367^{-10}	2.1904^{-10}	2.0852^{-10}	1.9891^{-10}	1.8366^{-10}
3-4	2.8242^{-10}	2.8088^{-10}	2.7216^{-10}	2.5664^{-10}	2.4345^{-10}	2.2329^{-10}
5-6	4.7198^{-10}	4.4944^{-10}	4.2119^{-10}	3.8621^{-10}	3.6067^{-10}	3.2484^{-10}
7-6	8.4227^{-10}	8.1237^{-10}	7.7026^{-10}	7.1442^{-10}	6.7196^{-10}	6.1063^{-10}
7-8	1.3094^{-09}	1.2500^{-09}	1.1744^{-09}	1.0797^{-09}	1.0101^{-09}	9.1177^{-10}

3. CONCLUSIONS

This work offers atomic data for the Zn-like W ions. We have calculated energy levels, radiative transition probabilities among the fine structure levels. Partial and total collision strengths and excitation rate coefficients have been computed for the following representative temperatures: 500, 700, 1000, 1500, 2000, 3000 eV. Regarding the spectra, the theoretical wavelengths obtained range between 1.1868 nm and 358.9054 nm. The majority of the lines have been identified as belonging to electric dipole transitions.

But, in order to properly exploit complex spectra of these elements our theoretical data must be associated with experimental results. It is our hope that these results will be of significant use in plasma modelling.

3. REFERENCES:

[1]R. D. Cowan, "The Theory of Atomic Structure and Spectra", University of California Press, Berkeley, 1981.

[2]H.L. Zhang, D. H. Sampson and C. J. Fontes, Atomic Data Nucl. Data Tables 48 91 (1991)

[3]K. M. Aggarwal, F. P. Keenan, P. H. Norrington, S. J. Rose, Atomic Data for Modelling of Lasers, Central Laser Facility Annual Report 2000/2001.

[4]K. B. Fournier, Atomic Data Nucl. Data Tables 68 1 (1998).