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Electric dipole transition parameters for $2s3l3l'$- and $2p^5 3l3l'$-$3l$ (l, l'=0, 1, 2) transitions in W^{63+}

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ABSTRACT

Energy levels and electric dipole (E1) transition parameters such as wavelengths, transition probabilities and oscillator strengths from the levels of $2s3l3l'$ and $2p^5 3l3l'$ to $3l$, (l, l'=0, 1, 2), in highly ionized tungsten (W^{63+}, Na-like) have been reported. Highly ionized tungsten data are important, especially in the diagnostics of fusion energy devices and in astronomy. Calculations have been carried out from configuration interaction (CI) calculations using AUTOSTRUCTURE code (developed by Badnell) which includes Breit interactions and quantum electrodynamics (QED) contributions. The results obtained have been compared with other available works.

1. Introduction

Sodium-like highly-charged ions play an important role in the diagnostics of fusion energy devices [1] and in astronomy [2]. Spectrum of Na-like ions is also important for X-ray laser modeling and their dielectronic satellite spectra is of interest in L-shell diagnostics of very high-temperature laboratory plasmas such as future ITER (International Thermonuclear Experimental Reactor fusion plasmas). Also, among many-electron systems, ions with only a few valence electrons outside the last closed shell are the simplest, and those high-Z ions isoelectronic to sodium therefore present an excellent model for studying atomic calculations.

The number of works on tungsten ions can be found at the NIST [3]. Ionization energies of tungsten ions were presented by Kramida and Reader [4]. Feldman et al. [1] investigated the possible use of spectral lines from highly ionized tungsten ions to measure physical properties of ITER plasmas. They calculated the energy levels, Einstein coefficients for spontaneous radiation and collision rates for all the W ions using FAC code (Flexible atomic code). Ralchenko et al. [5] reported detailed analysis of extreme ultraviolet (EUV) spectra of highly-charged tungsten ions $W^{54+} - W^{63+}$ obtained with an electron beam ion trap (EBIT). Pütterich et al. [6] investigated modeling of measured tungsten spectra from ASDEX Upgrade and predictions for ITER. Biedermann et al. [7] reported spectroscopy of highly charged tungsten ions relevant to fusion plasmas. Energy levels and spectral lines of tungsten, W III through W LXXIV, were studied by Kramida and Shirai [8]. Gillaspy et al. [9] presented the first observation of the $3s_{1/2}$–$3p_{1/2}$ and $3s_{1/2}$–$3p_{3/2}$ resonance lines which known D-line doublet of Na-like W^{63+}. Excitation energies, radiative and autoionization rates, dielectronic satellite lines and dielectronic recombination rates for excited states of Na-like W were calculated by Safronova et al. [10]. Clementson and Beiersdorfer [11] measured the wavelengths of $n=3$ to

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$n=3$ transitions in highly charged tungsten ions including Na like tungsten. A large-scale relativistic configuration-interaction calculation of the $n=3$-3 transition energies for Ne- to Ar-like tungsten was carried out by Chen and Cheng [12]. A comprehensive theoretical study of atomic characteristics of ten tungsten ions in a broad range of wavelengths, energy levels and transition probabilities was presented by Hu et al. [13]. Beiersdorfer et al. [14] observed several inner-shell collisional satellite lines associated with oxygen-like, fluorine-like, sodium-like and magnesium-like. Transition energies of the D lines in Na-like ions were reported by Gillaspy et al. [15]. Dipti et al. [16] calculated L-shell electron excitations of Mg- through O-like tungsten ions. Also there are early works in the literature for Na-like ions including W^{63+} [17–21].

In this work, we have reported a large-scale calculations include energies for levels and electric dipole transition parameters for all transitions from the levels of *2s3l3l'* and *$2p^5$3l3l' (l, l'=0, 1, 2)* to the levels of *3 s, 3p* and *3d* in Na-like tungsten (W^{63+}, Z = 74) using AUTOSTRUCTURE code [22]. W^{63+} has the ground-state configuration of [Ne]3 s. Calculations include QED (self-energy and vacuum polarization) and Breit interaction (magnetic interaction between the 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. In addition, the electron correlation effects due to the Coulomb interaction between the electrons are also important, in particular, on fine structure and transitions. We have here taken into account the configurations including one-electron excitation from valence to other high sub-shell and one-electron excitation from *2 s* and *2p* subshell to other high subshells: *3 s, 3p, 3d, 2p3s^2, 2p3s3p, 2p3s3d, 2p3p^2, 2p3p3d, 2p3d^2, 2s3s^2, 2s3s3p, 2s3s3d, 2s3p^2, 2s3p3d* and *2s3d^2* . Therefore *1s^2* is fixed calculations through. In addition, *2p3l3l'* have been briefly taken instead of *$2p^5$3l3l'* in text and tables.

2. Calculation method

AUTOSTRUCTURE code [22,23] which is based on SUPERSTRUCTURE [24], is a general program for the calculation of atomic properties such as energies, radiative and autoionization rates and photoionization cross sections using non-relativistic or semi-relativistic wavefunctions. 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. In addition AUTOSTRUCTURE code uses non-relativistic or kappa-averaged relativistic wavefunctions and the full Breit interaction in Pauli approximation. This code also includes quantum electrodynamics (QED) contributions. More detailed information on the method of this code can be found in [22,23,25].

For an ion with N electrons, a set of configurations

$$c = \prod_{nl} (nl)^{q_{nl}}, \qquad \sum_i q_i = N \tag{1}$$

defines a trial solution $\Psi(\gamma)$ to a suitable Hamiltonian H in the multiconfigurational sum form

$$\Psi(\gamma|\mathbf{x}_1, \ldots \mathbf{x}_N) = \sum_k a_k \Phi_k(c_k(\gamma)|\mathbf{x}_1, \ldots \mathbf{x}_N) \tag{2}$$

where γ denotes configuration and coupling scheme. In intermediate coupling (IC) wave functions can be written as

$$\Psi = \Psi\left(\Gamma SLJM_J|\mathbf{x}_1, \ldots \mathbf{x}_N\right) \tag{3}$$

which are eigenvectors to the Breit–Pauli matrix $\langle k|H_{BP}|k'\rangle$ with eigenvalues E_k.

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. The contributions from Breit interaction and QED effects consisting of vacuum polarization and self-energy are added as a perturbation correction, in generally. Orbitals are fixed, but the mixing coefficients are calculated by diagonalizing the modified Hamiltonian. The correlation effects are taken into account by CI (configuration interaction) method. The correlation contribution should be separated for three parts: correlation of core electrons, correlation between core and valence electrons, and correlation of two valence electrons.

For transitions, this code computes Einstein coefficients and associated quantities for multipole transitions of low multipolarity (for electric dipole, E1, radiation). Generally, electric multipole transitions exist in both of LS coupling and intermediate coupling (or jj-coupling). Electric quadrupole (E2) and magnetic dipole (M1) transitions come into their own only in intermediate coupling. As intermediate coupling wave functions contain admixtures of order α^2, radiative operators must also be expanded up to Breit contributions order. In the long wavelength low intensity approximation the probability for spontaneous emission by E1 radiation,

$$A_{i'\to i} = 2.6774 \times 10^9 \frac{(E_i - E_{i'})^3}{g_i} \cdot S(i, i') \tag{4}$$