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Theoretical level energies and transition data for $4p^64d^4$, $4p^64d^34f$ and $4p^54d^5$ configurations of W^{34+} ion

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ABSTRACT

The *ab initio* quasirelativistic approach developed specifically for the calculation of spectral parameters of highly charged ions was used to derive transition data for the tungsten ion W^{34+}. The configuration interaction method was applied to include electron correlation effects. The relativistic effects were taken into account in the Breit–Pauli approximation. The level energies, radiative lifetimes τ, Landé g-factors are determined for the ground configuration $4p^64d^4$ and two excited configurations $4p^64d^34f$ and $4p^54d^5$. The radiative transition wavelengths λ and emission transition probabilities A for the electric dipole, electric quadrupole, electric octupole, magnetic dipole, and magnetic quadrupole transitions among the levels of these configurations are produced.

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Contents

1. Introduction

In the present work we continue our theoretical studies [1–3] of multicharged tungsten ions with an open 4d shell in the ground configuration. The unique physical properties of metallic tungsten empower the use of tungsten in high temperature devices [4,5]. Although tungsten ions of different ionization degrees are investigated by both experimental and theoretical methods for more than ten years [6–11], the atomic data needs remain unfulfilled [12,13] including the radiative properties in the visible and X-ray wavelength ranges.

A wide compilation of the spectroscopic data for the tungsten ions was published [14]. It is evident from that review that the tungsten ions that have an open 4d-shell are investigated very seldom. Only a few level energies of the ground configuration $4p^64d^4$ in W^{34+} are known experimentally. Other values of the level energies for this configuration are determined by semi-empirical methods. Moreover, the level energies of the lowest excited configurations $4p^54d^5$ and $4p^64d^34f$ are undetermined for this tungsten ion neither by experiment nor by theoretical methods.

The spectrum of the W^{34+} ion was investigated using several well-established theoretical approaches such as multiconfiguration Dirac–Fock (MCDF) or Dirac–Fock–Slater (DFS) [11,15,16]. Unfortunately, these studies consider only the ground configuration of W^{34+}, presenting level energies and radiative transition parameters. Nevertheless, their results can serve as benchmark data to evaluate accuracy of our theoretical results. In the previous work [10] the radiative transitions from the exited configuration levels were also considered using relativistic Dirac–Fock approximation, but their results were presented only in graphical plots with no numerical data. Similar way to present data is chosen in Ref. [9]. For that reason, although their results provide a nice qualitative insight into the spectra formation in the W^{34+} ion, it is a rather complicated task to use the results from Refs. [9,10] for the data evaluation or spectra modeling purposes. Experimental data for the magnetic dipole (M1) transitions among the ground configuration $4p^64d^4$ levels and few electric dipole (E1) transitions from the excited configuration $4p^64d^34f$ are listed in Ref. [7] along with theoretical results obtained using a relativistic HULLAC code. In addition, only one calculated wavelength value for a transition from the configuration $4p^54d^5$ is listed in their table.

The purpose of the present work is to determine the level energies, their radiative lifetimes, and the spectroscopic parameters of electric dipole (E1), electric quadrupole (E2), electric octupole (E3), magnetic dipole (M1), and magnetic quadrupole (M2) transitions among the levels of the ground and also of two excited configurations. Calculated data can facilitate experimental studies of corresponding spectra as we extend previous data sets for the W^{34+} ion by including levels of the excited configurations $4p^54d^5$ and $4p^64d^34f$. On the other hand, these data can be adopted directly for plasma spectra modeling. As in our previously investigated W^{37+}, W^{36+} and W^{35+} ions, we utilize a quasirelativistic approach (QR) with a comprehensive inclusion of correlation effects to investigate the spectroscopic properties of the W^{34+} ion.

In Section 2 we provide a description of the adopted QR approximation. Since this approximation completely matches one applied in our previous calculations of highly-charged tungsten ions, here we present only a short summary of our method. The determined results and their accuracy assessment are discussed in Section 3.

2. Calculation method

We use the quasirelativistic approximation in our *ab initio* calculation of the level energies and radiative transition parameters, such as transition line strengths S, weighted oscillator strengths gf, radiative multipole transition probabilities A (transition rates). The most complete and consistent description of our method utilized to calculate the spectroscopic parameters in the quasirelativistic approach is given in Ref. [17].

At the very start, the radial orbitals (RO) are obtained by solving the quasirelativistic Hartree–Fock (QRHF) equations [18,19] for the one-electron RO in the ground configuration $4p^64d^4$. In this way we determine RO for the 1s, 2s, 2p, 3s, 3p, 3d, 4s, 4p, and 4d electrons. Then the QRHF equation for the 4f electron is solved in a frozen-core potential for the $4p^64d^34f$ configuration. The virtually excited electrons with $n > 4$ are described by the quasirelativistic transformed radial orbitals (TRO). The method to determine the quasirelativistic TRO with two variational parameters was presented in [17]. TRO are determined for the radial orbitals with the principal quantum number $5 \le n \le 9$ and with all possible values of the orbital quantum number $l < n$.

These quasirelativistic RO and TRO are utilized to describe electrons in all configurations of both even and odd parity. Such an identical RO basis enables us to avoid the non-orthogonality problems of RO when the radiative transition parameters among the levels of different parity or the electron-impact excitation data are calculated. For the calculation of the level energies, the one-electron and the two-electron relativistic corrections are included in the Breit–Pauli approximation, as it is standard in our calculations.

The correlation corrections are included by implementing the configuration interaction (CI) method. The CI wavefunction expansion is based on the set of admixed configurations that are produced by promoting one or two electrons from the $4l$ shells of the adjusted (investigated) configurations to all states possible from the generated RO basis.

The admixed configurations produced by promoting electrons to other $4l$ shells are listed in Table A. The inclusion of these configurations in the CI wavefunction expansion is important as they are energetically close to the adjusted ones. Although non-diagonal matrix elements of the energy operator for these configurations are not very large, their contribution to the correlation energy remains substantial.

Significantly longer list of the admixed configurations is produced when the $4l$ electrons are promoted to the shells described

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