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High-accuracy multi-configuration Dirac–Hartree–Fock calculations of the energy levels and transition properties of Ga-like to Br-like gadolinium ions

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HIGHLIGHTS

- A complete and accurate data set of excitation energies, lifetimes, wavelengths and E1, M1, E2, M2 and E3 line strengths, transition rates, and oscillator strengths for Ga-like to Br-like Gd ions is reported.
- The Multi-configuration Dirac–Hartree–Fock method is employed.
- The effects of core–valence electron correlation from the deep subshells 3*d* and 3*p* have been investigated.
- The computed excitation energies from the present MCDHF calculations of the VV + CV_{3d} + CV_{3p} model agree well with the experimental values. The differences are less than ±0.1% for most of the levels.

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ABSTRACT

Theoretical calculations of Ga-like to Br-like gadolinium ions were performed by using the fully relativistic multi-configuration Dirac–Hartree–Fock (MCDHF) method. Extensive lists of excitation energies, wavelengths, line and oscillator strengths, and E1, M1, E2, M2, and E3 transition rates are presented. The effects of core–valence electron correlation from the deep subshells 3*d* and 3*p* are investigated and the accuracy of the results is confirmed by comparing with available theoretical and experimental data sets.

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Contents

1. Introduction

As the potential light source for future semiconductor lithography [1], gadolinium has drawn a lot of attention due to its strong emitted lines around 6.7 nm [2–4] in the form of an unresolved transition array. Since the mixture of gold–gadolinium material could improve the Rosseland mean opacity and provide higher laser to x-ray conversion efficiencies [5–8], gadolinium is also proposed as hohlraum wall material in the indirect laser drive of inertial confinement fusion (ICF). Thus an extensive amount of atomic structure data for Gd ions with different ionization degrees are needed for modeling and diagnosing ICF plasmas parameters.

The resonance transitions of $n = 4 \rightarrow n = 4$ for different Gd ions were measured using the electron-beam ion trap (EBIT) at the National Institute of Standards and Technology (NIST) [9], the Large Helical Device at the National Institute for Fusion Science (NIFS) [10–13] and other equipments [14–20]. For the gadolinium ions from Ga-like to Br-like systems, which are considered in the present work, 73 lines were identified [21,22]. Using the FAC code [23], the theoretical energies and transition wavelengths for these 73 transitions were also reported in the Refs. [21,22]. The experimental and theoretical values for few transitions of the gadolinium ions from Gd^{+33} to Gd^{+29} were also provided by different studies [24,25].

In the present work, we provide the elaborate *ab initio* calculations of atomic properties of Ga-like Gd^{33+} to Br-like Gd^{29+}, which is a continuation of our recent work [26–30] of providing complete data of energy levels and transition characteristics for L-, M-, and N-shell ions to the accuracy needed to analyze new observations from different sources, and to model and diagnose fusion plasmas. By using the MCDHF method [31,32] and the subsequent relativistic configuration interaction (RCI) approach implemented in the GRASP2K package [33,34], a consistent and highly accurate data set of energy levels, lifetimes, wavelengths, and E1, E2, M1, M2 and E3 line strengths, transition rates, and oscillator strengths for the gadolinium ions from Ga-like to Br-like systems is provided. The impact of core–valence correlation with deeper subshells and the convergence of spectral data is analyzed. The uncertainties of our MCDHF/RCI calculations are smaller than 0.1% for almost all the available observed transition wavelengths.

2. Theory and calculations

In the MCDHF method, the Dirac–Coulomb Hamiltonian was defined as

$$H_{\mathrm{DC}} = \sum_{j=1}^{N}[\boldsymbol{\alpha}_j \cdot \boldsymbol{p}_j + \beta_j c^2 + V_{nuc}(r_j)] + \sum_{j<k}\frac{1}{r_{jk}}\,, \tag{1}$$

where $V_{nuc}(r_j)$ is the potential from a two parameter Fermi nuclear charge distribution and r_{jk} is the distance between electrons j and k. An electronic state of the ion is represented by an atomic state function (ASF) $\Psi(\gamma J)$, which is expanded in terms of configuration state functions(CSFs)

$$\Psi(\gamma J) = \sum_{i=1}^{n} c_i \Phi(\gamma_i J)\,. \tag{2}$$

The CSFs are built from products of one-electron Dirac orbitals [35]. Based on the extended optimal level (EOL) scheme [36], the radial parts of the Dirac orbitals and the expansion coefficients of the targeted states are all optimized to self-consistency by solving the MCDHF equations, which are derived using the variational approach. The zero-frequency limit of the Breit interaction and the leading part of the QED effects (self energy and vacuum polarization) are taken into account in the subsequent RCI calculations.

The odd and even parity states are determined in two separate calculations. We start this calculation without any excitation from the reference configurations which is usually referred to as the Dirac–Hartree–Fock (DHF) calculation as the first step. The reference configurations are the $4s^2(4p, 4d, 4f)$, $4s4p^2$, $4s4p4d$, $4p^3$ configurations for the Ga-like Gd ion, and are the $4s^24p^k$, $4s^24p^{k-1}4d$ and $4s4p^{k+1}$ configurations with $k = 2, 3, 4$, and 5 for Ge-like, As-like, Se-like, and Br-like Gd ions, respectively. Subsequently, the CSFs expansions are obtained through single and double excitations from the shells of the reference configurations up to a

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