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Calculation of energy levels, lifetimes and radiative data for La XXIX to Sm XXXIV

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HIGHLIGHTS

- Lowest 27 levels for La XXIX to Sm XXXIV are calculated.
- Radiative data for E1, E2, M1 and M2 transitions within lowest 27 levels are presented.
- Effect of nuclear charge on the transition wavelength of allowed EUV transitions is studied graphically.
- Effect of nuclear charge on transition probability of allowed EUV transitions is studied graphically.
- Lifetimes for lowest 27 fine structure levels are provided.

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ABSTRACT

We present the most comprehensive atomic data for La XXIX to Sm XXXIV with single electron excitation from M-shell to N-shell and N-shell to higher shells. We have presented energy levels, lifetimes and radiative data using Multi-configuration Dirac–Fock (MCDF) method for the lowest 27 states belonging to the configuration $3d^{10}4l$ ($l = 0, 1, 2, 3$), $3d^{10}5l$ ($l = 0, 1, 2, 3, 4$), $3d^{10}6l$ ($l = 0, 1, 2, 3, 4$) and $3d^{9}4s^{2}$. We have also considered relativistic effects by incorporating quantum electrodynamics (QED) and Breit corrections. We have made comparisons of our presented results with available theoretical as well as experimental results and a good agreement is achieved. Further, we have also reported energy levels by performing distorted wave calculations with fully relativistic flexible atomic code (FAC). The calculations match well with MCDF results. Additionally, we have investigated the effect of nuclear charge on transition wavelength and radiative rates for strong Extreme Ultraviolet (EUV) transitions from $n = 4 \rightarrow 4$. We believe that our reported data in this work may be useful in various applications of lanthanide ions related to broad area of research such as applied physics, laser physics and astrophysics etc.

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Contents

1. Introduction

In the last few years, the spectroscopic study of high-Z highly charged ions has become the topic of considerable interest. Since the rare earth elements have a lot of applications in the field of optoelectronics to detect and control light, and in astrophysics for examining the growth of peculiar stars due to the large number of their radiative characteristics. Therefore, the spectra of lanthanide atoms or ions are of particular interest related to elemental research in several areas of applied physics and astrophysics. Also, many significant experimental and theoretical works on neutral rare earth elements have been published and available in the National Institute of Standards and Technology (NIST) Atomic Spectra Database [1]. To the best of our knowledge, there is only a limited amount of radiative data for higher excited states are available in the literature for highly charged lanthanide ions. Hence, in the present paper, we have provided the radiative data for first six Cu-like lanthanide ions.

In the past few decades, various experiments as well as theoretical computations on Cu-like lanthanide ions have been carried out by implementing various methods. Early, Carlson et al. [2] has provided the ionization potentials for Cu-like La to Sm and for other highly charged ions. Energy levels, wavelengths and transition probabilities of electric dipole (E1) transitions for Cu-like ions including lanthanide ions have been reported by Cheng et al. [3] by applying the Hartree–Fock method. Curtis [4] has listed the fine-structure separations of $^2P^o$ and ^2D for Cu isoelectronic sequence. Reader et al. [5] has measured wavelengths for Ba^{27+} to W^{45+} including La^{28+}, Nd^{31+} and Sm^{33+} by implementing the technique of laser produced plasma. Curtis [6] has reported the fine structure intervals for several multiply charged ions including Cu-like ions. Doschek et al. [7] has measured the EUV (extreme ultra-violet) and X-ray transition wavelengths of Cu-like Sm and other ions using laser produced plasmas. Ionization limits and wavelengths of Cu-like ions have been calculated by using ab initio method by Tragin et al. [8]. Further, Curtis et al. [9] has reported lifetimes of levels belonging to $3d^{10}$ 4p and $3d^{10}$ 4d of Cu isoelectronic sequence. Finkenthal et al. [10] has observed the transition $4s_{1/2}$ to $4p_{1/2}$ of Cu-like Sm in tokamak plasmas. Wavelengths for some transitions of Cu-like Sn, Xe, La, Nd, Eu, Gd, Dy, and Yb have been provided in the literature by Seely et al. [11]. Seely et al. [12] provided wavelengths of 18 strongest transitions for Cu isoelectronic sequence by employing MCDF method as used in our work, but using optimal level (OL) scheme. Zhang et al. [13] has calculated the collision and oscillator strengths for Cu-like ions including Cu-like Nd, Pm and Sm using relativistic distorted wave method. The energies of the first three levels of Cu-like ions with atomic number $Z = 29$–92 have been computed by Johnson et al. [14] by employing relativistic many body perturbation theory (RMBPT). Resonance transition energies are determined by Kim et al. [15] for Cu-like and other ions. Recently, Podpaly et al. [16] has identified EUV transitions for Cu-like Sm and other highly charged Sm and Er ions at the NIST electron beam ion trap (EBIT).

Although a variety of papers have been published in the literature, there is a lack of complete and definite atomic data for highly charged lanthanide ions. The application of rare earth elements in the origin of light sources for the next generation for EUV lithography and in astrophysics requires a complete radiative data for highly charged rare earth elements which opens the door for the additional study in this area. Hence, in this work, we have presented the complete radiative data for the lowest 27 levels of first six Cu-like lanthanides ions along with lifetimes and energy levels. From the theoretical point of view, various electronic properties of the system changes with the increase of nuclear charge along the isoelectronic sequence. Therefore, we have also studied the effect of increase of nuclear charge on transition probabilities and transition wavelengths belonging to allowed strong EUV transitions within $n = 4$ shell.

2. Theoretical method

To execute these extensive calculations, we have adopted a fully relativistic MCDF method applied in General purpose relativistic atomic structure package (GRASP). This method was developed by Grant et al. [18] and improved by Norrington [17] and has been successfully applied in our previous works [19–30]. The contributions from Breit interactions as well as QED corrections as a first order perturbation theory have been also included. Since the comprehensive and elaborate explanation of this method has been presented elsewhere [18,31–34], so only a brief synopsis of this method is reviewed here. To calculate radial wave functions, we have opted scheme of extended average level (EAL) in which weighted trace of the Hamiltonian matrix is minimized. For N electron atom or ion, Dirac–Coulomb Hamiltonian in MCDF method is given by

$$\hat{H}^{DC} = \sum_{i=1}^{N} \hat{H}_i + \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \frac{1}{|\hat{r}_i - \hat{r}_j|}, \tag{1}$$

where the one-electron Hamiltonian $\hat{H}_i$ is given by

$$\hat{H}_i = c\vec{\alpha}_i \cdot \vec{p}_i + \beta mc^2 + V_{nuc}. \tag{2}$$