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Energy levels, lifetimes and radiative rates for transitions in the bromine isoelectronic sequence La XXIII-Dy XXXII, W XL

K. Wang [a,b], C.Y. Zhang [c], R. Si [c], S. Li [d], Z.B. Chen [e,f,*], X.H. Zhao [a], C.Y. Chen [c,**], J. Yan [d,**]

[a] Hebei Key Lab of Optic-electronic Information and Materials, The College of Physics Science and Technology, Hebei University, Baoding 071002, China
[b] Group for Materials Science and Applied Mathematics, Malmö University, SE-20506, Malmö, Sweden
[c] Shanghai EBIT Lab, Institute of Modern Physics, Department of Nuclear Science and Technology, Fudan University, Shanghai 200433, China
[d] Institute of Applied Physics and Computational Mathematics, Beijing 100088, China
[e] College of Science, National University of Defense Technology, Changsha 410073, China
[f] School of Science, Hunan University of Technology, Zhuzhou 412007, China

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ABSTRACT

Using the multiconfiguration Dirac–Fock method, calculations for the lowest 62 levels of the ([Ar] $3d^{10}$)$4s^2 4p^5$, ([Ar] $3d^{10}$)$4s^2 4p^3 4d^2$, ([Ar] $3d^{10}$)$4s^2 4p^4 4d$, ([Ar] $3d^{10}$)$4s4p^6$, and ([Ar] $3d^{10}$)$4s4p^5 4d$ configurations are performed for the bromine isoelectronic sequence La XXIII-Dy XXXII, W XL. Results of energy levels, lifetimes, wavelengths, and electric dipole, magnetic dipole, electric quadrupole, and magnetic quadrupole radiative rates are presented. In order to assess the accuracy of results, independent calculations for W XL have been carried out using the many-body perturbation theory (MBPT) method. Comparisons are made with available theoretical results from other calculations and the observed values of the Atomic Spectra Database of the National Institute of Standards and Technology. Energy levels are estimated to be accurate to better than 1%, and radiative rates (and lifetimes) are accurate to better than 20% for a majority of strong transitions. These results should be useful in many applications of lanthanide ions related to broad area of research such as applied physics, laser physics and fusion science.

* Corresponding author at: College of Science, National University of Defense Technology, Changsha 410073, China.
** Corresponding authors.
E-mail addresses: chenzb008@qq.com (Z.B. Chen), chychen@fudan.edu.cn (C.Y. Chen), yan_jun@iapcm.ac.cn (J. Yan).

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Contents

1. Introduction

Rare earth elements are important in astrophysics in relation to nucleosynthesis and star formation [1], as many of their lines from different ionization stages are frequently observed. These spectral lines provide information on physical condition and chemical abundances of the sources. To interpret these observations and obtain physical condition of the astrophysical plasmas, the knowledge of accurate atomic data, such as energy levels, transition rates, and lifetimes, are required. Rare earth elements also play a critical role in many high-tech applications ranging from photovoltaic devices, medical imaging technology, lighting, atomic clocks to catalysts and so on [2]. It is indispensable to carry out a comprehensive investigation on atomic structures and transition properties of these elements.

A considerable number of contributions both experimentally and theoretically have been devoted to the determination of atomic properties for rare earth elements. In respect of experiment, Gayasov et al. [3] measured the spectrum of La VIII in the 80−1240 Å wavelength region. Using a variety of normal and grazing incidence spectrographs, the spectrum of the $(5p^2+5s5d+4f5p)\rightarrow(5p5d+4f5d+5s5f)$ transitions for La X were analyzed by Ryabtsev et al. [4]. Tauheed et al. [5] measured the spectrum of La VIII in the wavelength region 80−1220 Å using a triggered spark light source. Furmann et al. [6] reported experimental results of fine and hyperfine structures for electronic levels belonging to even configurations in the lanthanum atom. Hyperfine structures of La I lines were investigated by Siddiqui et al. [7] using laser optogalvanic spectroscopy in a hollow cathode discharge lamp. Gamper et al. [8] reported the new even-parity fine structure levels of the Lanthanum atom discovered by means of optogalvanic spectroscopy. Podpaly et al. [9] reported spectroscopic measurements of highly charged samarium and erbium performed at the Electron-Beam-Ion-Trap (EBIT). They observed 71 lines from Kr-like Sm^{26+} to Ni-like Sm^{34+}. There are also many other studies on rare earth elements [10–12]. In respect of theory, Zhong et al. [13] reported the energy levels, transition probabilities, and electron impact collision strengths for La XXX. Li et al. [14] reported the calculations of energies and radiative rates for parity-forbidden transitions within the $4f^3$ configuration in La-like ions Pr^{2+} and Nd^{3+}. Karaçoban et al. [15] calculated wavelengths, weighted oscillator strengths, and transition probabilities for electric dipole transitions for some excited levels in neutral lanthanum using the multi-configuration Hartree–Fock (MCHF) method. Goyal et al. [2] reported the calculated energy levels, lifetimes, and radiative data for La XXIX to Sm XXXIV. Safronova et al. [16] reported relativistic many-body calculation of energies, transition rates, and lifetimes in Cs-like La III. They also carry out a comprehensive study of higher-order correlation effects to the excitation energies of La, La^+, Ce, Ce^+, Ce^{2+}, and Ce^{3+}.

Although some efforts regarding rare earth elements have been expended in the past, there is, a lack of complete and definite atomic data for bromine isoelectronic sequence. The laboratory analyses are still extremely fragmentary or even missing for many