Atomic Data and Nuclear Data Tables 107 (2016) 367–405

Contents lists available at ScienceDirect

Atomic Data and Nuclear Data Tables

journal homepage: www.elsevier.com/locate/adt

Energy levels and radiative transition rates for Ba XLVIII

Indu Khatri [a,*], Arun Goyal [a], Sunny Aggarwal [a,c], A.K. Singh [b], Man Mohan [a]

[a] Department of Physics and Astrophysics, University of Delhi, Delhi 110007, India
[b] Department of Physics, D.D.U. College, University of Delhi, Delhi 110015, India
[c] Department of Physics, Shyamlal College, University of Delhi, Delhi 110032, India

HIGHLIGHTS

- Lowest 431 levels of Ba XLVIII are calculated.
- Radiative data for E1, E2, M1 and M2 transitions from the lowest 3 levels to 431 levels are presented.
- Lifetimes for lowest 431 fine structure levels are provided.

ARTICLE INFO

Article history:
Received 6 April 2015
Received in revised form
8 June 2015
Accepted 10 July 2015
Available online 29 July 2015

Keywords:
Energy levels
Radiative rates
Lifetimes
Transition wavelengths
Oscillator strengths
Configuration interaction

ABSTRACT

Energy levels and radiative rates are reported for transitions in F-like Ba XLVIII. Configuration interaction has been included among 27 configurations (generating 431 levels) over a wide energy range up to 618 Rydbergs, and the fully relativistic multi-configurational Dirac–Fock method adopted for the calculations. To assess the accuracy, calculations have also been performed with the flexible atomic code, FAC. Radiative rates, oscillator strengths and line strengths are reported for all electric dipole, magnetic dipole, electric quadrupole, and magnetic quadrupole transitions from the lowest 3 levels, although calculations have been performed for a much larger number of levels. We have made comparisons of our results with existing available results and a good agreement has been achieved. Additionally, lifetimes for all 431 levels are listed.

* Corresponding author.
E-mail address: indu.khatri.du@gmail.com (I. Khatri).

http://dx.doi.org/10.1016/j.adt.2015.07.002

Contents

1. Introduction

In engineering applications, barium was initially used in high-temperature superconductors [1], electro-vacuum devices and more recently in gas lasers [2]. In fundamental research, spectra of Ba ions have been investigated in almost every electron beam ion trap (EBIT). In the electron gun cathode of EBITs, barium is used as a dopant. Therefore, ions of Ba migrate into the trap region after being emitted from the cathode and display spectra along with those of other elements. Spectra of Ba ions in the visible region have been reported from the Livermore EBIT [3,4] group. Also using many EBITs, X-ray and EUV region spectra have been investigated.

The study of highly charged ions is given much attention due to their importance for various fields such as the diagnostics of plasmas, laser physics and astrophysics. Highly charged ions are found to exist in a number of high-temperature astrophysical sources emitting or absorbing radiation in the optical to X-ray range. Information about physical conditions and chemical abundances in the sources can be provided by the spectral lines of these ions. Accurate radiative data is required in the analysis and modeling of these spectra.

The data provided by spectral studies of ions of heavy elements are invaluable for atomic physics, astronomy and high-temperature plasma diagnostics. In particular, atomic data are required for diagnostic purposes as lines from fluorine-like ions have been observed in solar flares [5,6], planetary nebulas and laboratory plasmas [7,8]. The knowledge of accurate atomic parameters such as transition probabilities are crucial in estimating the densities of species in the stars, galaxies and nebulae atmospheres [9]. Forbidden lines in fluorine like ions are important as these are found to occur at long wavelengths and hence accurate line profiles are obtained. These lines have been used in the study of nonthermal mass motions occurring in solar corona. Many forbidden lines with np^k configuration of the fluorine isoelectronic sequence have been identified in tokamak discharges and in the solar corona and flares.

Various studies have been performed on fluorine-like ions. Hutton et al. [10] observed several transitions of the Ba XLVIII using an EBIT and the spectra were produced by exciting ions with a 10 keV electron beam. Feldman et al. [11] identified transitions of the type 2s-2p in the highly charged fluorine like Mo, Cd, In and Sn. These were used to produce extrapolated values for the Ba XLVIII transitions. Transition probabilities between levels of the $2s^22p^5$, $2s2p^6$, $2s^22p^43l$ and $2s2p^53l$ configurations using the relativistic distorted-wave method were calculated by Sampson et al. [12]. Ivanova and Gulov [13] calculated the three lowest energy levels using relativistic perturbation theory with a model potential. Kim and Huang [14] presented spin–orbit intervals in the ground state $2p^5\ ^2P_{3/2} - {}^2P_{1/2}$ of F-like ions for $Z \leqslant 56$. Rodrigues et al. [15] calculated atomic binding energies for the lithium to dubnium isoelectronic series in the Dirac–Fock approximation. Gu [16] used a combined configuration interaction and many-body perturbation theory approach to calculate the level energies of $1s^22l^q$ ($1 \leqslant q \leqslant 8$) states for ions with $Z \leqslant 60$. Cheng et al. [17] in 1979 obtained energy levels, oscillator strengths and transition probabilities for the first row atoms (Li through F) using the multiconfigurational Dirac–Fock method. Edlén [18] calculated transition energies for ions from $Z = 11$ to $Z = 33$ using a semi-empirical formula with three adjustable parameters. Some authors [19,20] calculated oscillator strengths of transition from the ground states of fluorine-like ions using the CIV3 code. Atomic data for fluorine-like iron was obtained by Nahar [21] using the relativistic Breit–Pauli approximation under the Iron Project. Energy levels and transition rates for low-lying states for ions up to Ti XIV using multiconfigurational Breit–Pauli wavefunctions were calculated by Fischer and Tachiev [22]. Recently, energy levels and transition probabilities among levels of the ground configuration and first 23 excited configurations of Fe XVIII using multiconfigurational Dirac–Fock method have been calculated by Jonauskas et al. [23]. Also, Jönsson et al. [24] calculated energies and electric dipole (E1), magnetic dipole (M1), and electric quadrupole (E2) transition rates for $2s^22p^5$ and $2s2p^6$ configurations states in F-like ions between Si VI and W LXVI.

As only limited work on Ba XLVIII is available, the aim of the present paper is to report a set of results for fluorine-like barium among 431 levels belonging to $2s^22p^5$, $2s2p^6$, $2s^22p^43l$, $2s2p^53l$, $2p^63l$, $2s^22p^44l$, $2s2p^54l$, $2s^22p^45l$ and $2s2p^55l$ configurations that can be confidently applied in plasma modeling and other astrophysical applications. Calculations have been performed using the fully relativistic multiconfiguration Dirac–Fock approach, which is one of the most standard methods suitable for predicting atomic data for transitions in highly charged ions or heavy atoms. Calculations have also been performed with the flexible atomic code (FAC) to assess the accuracy of results. We report radiative rates for all E1, E2, M1 and magnetic quadrupole (M2) transitions from lowest 3 levels to all 431 levels and also provide theoretical lifetimes for all levels. A comparison of our theoretical calculations with the data available from the National Institute of Standards and Technology (NIST) [25] database has been provided.

2. Theoretical method

We have adopted the multiconfiguration Dirac–Fock (MCDF) code to generate the wavefunctions, which was originally developed by Grant et al. [26] and updated by Norrington [27]. It includes higher order relativistic corrections arising due to Breit