

Energies, Wavelengths, and Transition Probabilities in Sc XIII

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Abstract—The fine-structure energy levels and lifetimes are calculated for the lowest 218 levels of the $2s^2 2p^5$, $2s 2p^6$, $2s^2 2p^4 3s$, $2s^2 2p^4 3p$, $2s^2 2p^4 3d$, $2s 2p^5 3s$, $2s 2p^5 3p$, $2s 2p^5 3d$, $2p^6 3s$, $2p^6 3p$, $2p^6 3d$, $2s^2 2p^4 4s$, $2s^2 2p^4 4p$, $2s^2 2p^4 4d$, $2s 2p^5 4s$, $2s 2p^5 4p$, and $2s 2p^5 4d$ configurations in Sc XIII using the general-purpose relativistic atomic structure package (GRASP). The atomic data of the electric dipole ($E1$), electric quadrupole ($E2$), magnetic dipole ($M1$), and magnetic quadrupole ($M2$) transitions from the levels of $2s^2 2p^5$, $2s 2p^6$, $2s^2 2p^4 3s$, $2s^2 2p^4 3p$, $2s^2 2p^4 3d$, $2s 2p^5 3s$, $2s 2p^5 3p$, $2s 2p^5 3d$, $2p^6 3s$, $2p^6 3p$, and $2p^6 3d$ configurations to the levels of the $2s^2 2p^5$ and $2s 2p^6$ configurations are presented. The GRASP results are compared with the other calculations and measurements.

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1. INTRODUCTION

The atomic data of highly ionized atoms are needed for several fields, such as astrophysics, laser physics, and plasmas physics. The magnetic-dipole transitions in the $2s^2 2p^5$ configuration are an important tool for the diagnostics of high-temperature plasmas [1]. The atomic data for ions in the F -like ions have been reported [1–23].

Cohen et al. [2] have observed the lines of the $2s^2 2p^5 - 2s^2 2p^4 3s$, $2s^2 2p^5 - 2s^2 2p^4 3d$, and $2s 2p^6 - 2s 2p^5 3s$ transitions of F -like ions from Sc XIII to Cu XXI. Chapman and Shadmi [3] have calculated the energy levels and oscillator strengths for transitions from the levels of the $2s^2 2p^4 3s$, $2s^2 2p^4 3d$, $2s 2p^5 3p$, $2p^6 3s$, and $2p^6 3d$ configurations to $2s^2 2p^5 P_{3/2}$, $2s^2 2p^5 P_{1/2}$ levels for the Sc XIII, Fe XVIII, and Cu XXI. The lines of the $2s^2 2p^5 - 2s^2 2p^4 3d$ transitions for the F -like ions with $19 \leq Z \leq 27$ have been observed by Feldman et al. [4].

The general-purpose relativistic atomic structure package code has been used in the calculation of the atomic data for transitions among the lowest 113 levels of the $2s^2 2p^5$, $2s 2p^6$, $2s^2 2p^4 3l$, $2s^2 p^5 3l$, and $2p^6 3l$ ($l = s, p, d$) configurations for F -like ions with $37 \leq Z \leq 53$ [19], and for ions with $55 \leq Z \leq 73$ [22]. Recently, Zhang et al. [23] have calculated the atomic data for $E1$, $E2$, $M1$, and $M2$ transitions between the lowest 200 levels of $2s^2 2p^5$, $2s 2p^6 3s$, $2s 2p^6 3p$,

$2s 2p^6 3d$, $2s 2p^6 4s$, $2s 2p^6 4p$, $2s 2p^6 4d$, and $2s 2p^6 4f$ configurations in Kr XXVIII.

In this work, we calculate the energy levels, lifetimes, wavelengths, transition probabilities, oscillator strengths, and line strengths for $E1$, $E2$, $M1$, and $M2$ transitions in Sc XIII using the general-purpose relativistic atomic structure package.

2. CALCULATION AND RESULTS

2.1. Energy Levels

The atomic data of Sc XIII of the lowest 218 levels of $2s^2 2p^5$, $2s 2p^6$, $2s^2 2p^4 3s$, $2s^2 2p^4 3p$, $2s^2 2p^4 3d$, $2s 2p^5 3s$, $2s 2p^5 3p$, $2s 2p^5 3d$, $2p^6 3s$, $2p^6 3p$, $2p^6 3d$, $2s^2 2p^4 4s$, $2s^2 2p^4 4p$, $2s^2 2p^4 4d$, $2s 2p^5 4s$, $2s 2p^5 4p$, and $2s 2p^5 4d$ configurations are calculated using the GRASP code [24].

In Table 1, we present the energy levels (in Ryd), and the mixing coefficients for 218 fine-structure levels of the $2s^2 2p^5$, $2s 2p^6$, $2s^2 2p^4 3l$, $2s 2p^5 3l$, $2p^6 3l$, $2s^2 2p^4 4l$, and $2s 2p^5 4l$ ($l = s, p, d$) configurations obtained from GRASP with and without Breit and QED effects for Sc XIII. The Breit and QED energies (GRASP^b) are lower than the corresponding Coulomb energies (GRASP^a) by up to 0.04 Ryd ($\sim 0.1\%$), except for the $2s^2 2p^5 P_{1/2}$ level is 0.01 Ryd ($\sim 3.2\%$). The comparison between the present energy levels results and the compiled data from NIST [25] shows the level orderings are the same and the differences are within 0.4%, except for the $2s 2p^6 S_{1/2}$ level is 2%.

The lifetime of excited level j is given by $1/(\sum_i A_{ji})$ and the summation includes A -values from all types

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