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Relativistic atomic structure calculations and electron impact excitations of Fe^{23+}

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ABSTRACT

Relativistic calculations using the multiconfiguration Dirac–Fock method for energy levels, oscillator strengths, and electronic dipole transition probabilities of Li-like iron (Fe^{23+}) are presented. A configuration state list with the quantum numbers nl, where $n=2$–7 and $l=s,p,d,f,g,h,i$ has been considered. Excitations up to three electrons and correlation contributions from higher orbitals up to $7l$ have been included. Contributions from core levels have been taken into account, EOL (extended optimal level) type calculations have been applied, and doubly excited levels are considered. The calculations have been executed by using the fully relativistic atomic structure package GRASP2K. The present calculations have been compared with the available experimental and theoretical sources, the comparisons show a good agreement between the present results of energy levels and oscillator strengths with the literature. In the second part of the present study, the atomic data (energy levels, and radiative parameters) have been used to calculate the excitation and deexcitation rates of allowed transitions by electron impact, as well as the population densities of some excited levels at different electron temperatures.

1. Introduction

The accurate atomic data of iron ions are needed for astrophysics, the physics of controlled fusion, and plasma diagnostic [1–5]. The importance of spectroscopic analysis of the astronomically abundance elements such as iron lies within that it reflects their average abundances in the Universe, iron is one of the most abundant elements and is an important constituent in the evolution of stars and gaseous nebulae. As well as, iron is the heaviest abundant element in the solar system which produces the strongest high temperature lines in the solar spectrum. Lyman-α and K_β X-ray satellites of Fe^{23+} have been observed as well. In addition, the radiative decays from the open K-shell to inner and outer shells in the highly ionized atoms such as Fe^{23+} radiate wavelengths in the X-ray spectral region consisting of a large number of fine structure lines [6–9]. The present work is a complementary to preceding studies especially those interested in the open K-shell transitions such as Refs. [10,11], where the radiative rates for the transitions $1s2s2p$–$1s^2 2s$, $1s2s3p$–$1s^2 3s$, and $1s2s3p$–$1s^2 3d$ have been presented for Li-like iron. Most of transition arrays between levels with $n \geq 3$ and the $1s2l3l$ levels are missed in the literature, all of these transitions are in the X-ray spectral region with wavelength range 1.58–2.50 Å, a wide range calculations of the transition arrays $1s2p3p$–$1s^2 nl$ where $n=2$–5, $l=p,f$ are reported in the preset work.

Li-like iron has been widely studied in the literature such as [12–19], where an accurate values for energy levels and oscillator strengths of most configurations before the ionization potential has been reported. Large scale calculations of energy levels and oscillator strengths of Li-like

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Fe XXIV have been performed by Nahar and Pradhan [20,21], the Breit–Pauli R-matrix method has been applied to a configuration set of orbitals nl where n takes values up to 10 and $l=s-i$. Natarajan et al. [22] evaluated calculations of X-ray wavelengths, weighted oscillator strengths, and radiative rates from double electron transitions in Li-like ions including Fe^{23+}. The multiconfiguration Dirac–Fock (MCDF) method has been used by Dong et al. [23] to study the quantum-electrodynamics (QED) effects in the atomic structure calculations of lithium isoelectronic sequence including Fe^{23+}, the same method has been used to calculate the transition wavelengths, electronic dipole transition probabilities, line strengths, and absorption oscillator strengths for the $2s$–$3p$, $2p$–$3s$, and $2p$–$3d$ transitions in Li-like ions with $Z=7$–30 [24]. Del Zanna [25] has compiled experimental observations and theoretical calculations of energy levels and wavelengths of Fe^{23+} using the collisional model and SUPERSTRUCTURE code (SS).

In the present work, an extensive calculation of level energies, radiative rates, and wavelengths of allowed transitions in Li-like iron (Fe^{23+}) has been executed using the multiconfiguration Dirac–Fock method (MCDF) as implemented in the relativistic atomic structure package GRASP2K [26,27]. The relativistic effects such as Breit Hamiltonian and quantum electrodynamics effects (QED) have been included within the configuration interaction (CI) procedure. High-lying level correlations are incorporated to adjust the used wave functions. The used configuration state list which includes all possible jj-coupled configuration state functions (CSFs) consists of all single and double excitations up to $7l$, and single, double, and triple excitations up to the $6l$ orbitals. In the second part of this study, the calculated atomic data (energy levels and oscillator strengths), in addition, the excitation energies and collision strengths from Ref. [28] have been applied to the collisional radiative model to compute the excitation and deexcitation rates as a function of electron temperature T_e using private computer code [29]. The population densities for levels belonging to lithium-like iron are calculated as well. The calculations have been carried out over a limited range of electron density N_e and at different electron temperatures $T_e=0.25$, 0.50, and 0.75 of ionization potential.

2. MCDF calculations

2.1. Theoretical method

The present calculations of atomic structure for Li-like iron have been executed using the multiconfiguration Dirac–Fock method [26,27]. This method is based on the Dirac–Coulomb Hamiltonian which takes the form

$$H_{DC}=\sum_{i=1}^{N}(c\alpha_i\cdot\mathbf{p}_i)+(\beta_i-1)c^2+V_i^N+\sum_{i>j}^{N}\frac{1}{r_{ij}} \tag{1}$$

where c is the speed of light in atomic units, α and β are the 4×4 Dirac matrices and V^N is the monopole part of the electron–nucleus Coulomb interaction. In the calculation of the nuclear potential the Fermi nuclear charge distribution has been used, i.e.

$$\rho_{nucl}(r)=\frac{\rho_0}{1+e^{(r-b)/a}}. \tag{2}$$

The charge-density-distribution parameters for the ^{56}Fe nucleus are taken from [30], and the Fermi nuclear charge distribution parameters as suggested in GRASP2K [27] are $b=4.166$ fm and $a=0.523$ fm. ρ_0 is a constant and is determined from the total charge

$$4\pi\int_0^\infty \rho(r)r^2\,dr=Ze. \tag{3}$$

The atomic states considered here are expressed as linear combinations of configuration state functions (CSFs), which approximate atomic states with given angular momenta (J) and parities (P):

$$\Psi(\gamma PJM)=\sum_{j=1}^{NCSFs}c_j\Phi(\gamma_j PJM) \tag{4}$$

where J and M are the angular quantum numbers, and γ_j represents the configuration and any other quantum numbers required to specify the state j. The transition parameters such as radiative rates and line strengths between two atomic states γPJM and $\gamma' P' J' M'$ can be expressed in terms of the transition matrix elements

$$\langle\Psi(\gamma PJ)|\hat{Q}_k|\Psi(\gamma' P' J')\rangle \tag{5}$$

where $\hat{Q}_k$ is an electric or magnetic multipole transition operator of any tensorial order. To calculate the transition parameters between two atomic state functions, which contain separately optimized orbital sets, biorthogonal transformation of the ASFs has been carried out [31]. To transform the many-electron amplitude into a sum of one-electron reduced matrix elements standard Racah-algebra has been applied [32].

2.2. Computational procedures

In the present study, the spectrum calculations of the Fe^{23+} ion are divided into even and odd groups having all possible angular momenta (J-values). Two approaches have been followed to reach convergence. First, the estimation of the radial orbitals by solving the Dirac equation in a Thomas–Fermi potential for a single reference configuration. The $1s^22s$ level is the reference configuration for even levels and the $1s^22p$ for odd levels, then allowing single (S), double (D), and triple (T) excitations to active set of orbitals with $n=2$–6. This procedure generates a large number of configuration state functions (CSF), for example the number of generated CSFs by allowing single, double, and triple excitations for odd levels is 37,693 and 37,726 for even levels. The same computational procedures are exactly applied to the odd and even groups.

To get high accuracy in the case of a relatively heavy atom such as iron, a higher contribution should be expected from the similar levels [33]. This means that the contribution of the $7l$ shell is very important. To optimize the radial functions and expansion coefficients for a given list of configuration states, the self-consistent procedure (RSCF) including EOL type calculations (extended optimal