Theoretical Studies of Allowed (E1) and Forbidden (E2 and M1) Transitions in La IV

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The energies and lifetimes for $5p^6$, $5p^5nf$ ($n = 4$–10), $5p^5np$ ($n = 6$–10), $5p^5nh$ ($n = 6$–10), $5p^5nd$ ($n = 5$–10), $5p^5ns$ ($n = 6$–10), $5p^5ng$ ($n = 5$–10), and $5p^5ni$ ($n = 7$–10) configurations and the transition parameters for allowed transition (electric dipole E1), and forbidden transitions (electric quadrupole E2, and magnetic dipole M1) are presented for triply ionized lanthanum (La IV, $Z = 57$). The present results are obtained from a Hartree–Fock calculation with relativistic corrections and superposition of configurations (Cowan's HFR method) and general-purpose relativistic atomic structure package based on a fully relativistic multiconfiguration Dirac–Fock method. Comparisons are made with experimental and other available theoretical results to assess the reliability and accuracy of the present calculations. Moreover, some new wavelengths, oscillator strengths and transition probabilities of E1, E2, and M1 transitions have been obtained using these methods. These results are reported for the first time in this work.

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1. Introduction

The stellar spectra are generally dominated by neutral atoms and ions in low charge states. Lines of triply ionized lanthanides are also expected to appear in hot star spectra according to ionization equilibrium defined by the Saha equation. Because of a lack of atomic data, they have not yet been recognized and investigated [1].

The triply ionized lanthanum (La IV) belongs to the xenon isoelectronic sequence. Thus it is expected to have a typical rare-gas-like energy-level structure. Its ground state is $5p^6\ {}^1S_0$ and observed excited states are of the type $5p^5nl$. Available theoretical and experimental works on energy levels, radiative lifetimes, and transition parameters for La IV were reported in our previous works in detail [2, 3]. Studies of Epstein and Reader are the first investigations of spectra of La IV [4, 5]. The five resonance lines were reported in [4]. Later, they were able to determine 190 transitions and classify some excited levels [5]. $4d^{10}$–$4d^9nf$, np ($n = 6$–10) transitions were analyzed by Hansen et al. [6]. Biémont et al. carried out calculations of atomic structure and transition rates for La IV [1]. Excitation energies of La IV were calculated by Eliav and Kaldor [7]. Recently, Loginov reported transition probabilities and lifetimes for La IV experimentally and theoretically [8]. For La IV, it has been not presented a study about forbidden transition parameters. The data on forbidden transitions for this ion have been firstly presented in this work.

The aim of this paper is to obtain atomic data for triply ionized lanthanum (La IV, $Z = 57$) using relativistic Hartree–Fock (HFR) code [9] and general-purpose relativistic atomic structure package (GRASP) code [10]. We have reported relativistic energies, the Landé g-factors and lifetimes for the levels of $5p^6$, $5p^5nf$ ($n = 4$–10), $5p^5np$ ($n = 6$–10), $5p^5nh$ ($n = 6$–10), $5p^5nd$ ($n = 5$–10), $5p^5ns$ ($n = 6$–10), $5p^5ng$ ($n = 5$–10), and $5p^5ni$ ($n = 7$–10) configurations, and the transition parameters, such as the wavelengths, oscillator strengths, and transition probabilities, for electric dipole (E1), electric quadrupole (E2), and magnetic dipole (M1) transitions between excitation levels in La IV. Calculations have been carried out by the HFR method [11] and the GRASP atomic structure package based on a fully relativistic multiconfiguration Dirac–Fock (MCDF) method [12]. HFR method considers the correlation effects and relativistic corrections. These effects contribute importantly to the physical and chemical properties of atoms or ions, especially lanthanides. For valence excitations, we have only taken into account the configurations including one electron excitation from valence to other subshells: $5p^6$, $5p^5nf$ ($n = 4$–10), $5p^5np$ ($n = 6$–10), $5p^5nh$ ($n = 6$–10), $5p^5nd$ ($n = 5$–10), $5p^5ns$ ($n = 6$–10), $5p^5ng$ ($n = 5$–10), and $5p^5ni$ ($n = 7$–10) configurations outside the core [Cd] in La IV for the HFR calculation. The Breit interactions (magnetic interaction between the electrons and retardation effects of the electron–electron interaction) for relativistic effects, quantum electrodynamical (QED) contributions (self-energy and vacuum polarization) and correlation effects (valence–valence (VV), core–valence (CV), and core–core (CC)) which are important for electronic structure and spectroscopic properties of many electron

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systems, are included in MCDF method. In MCDF calculations, various configuration sets have been considered for correlation effects (including VV, CV, and CC correlations). In calculations, we have taken into account $5p^6$, $5p^5 6s$, $5p^5 4f$, $5p^5 5d$, $5p^5 6p$, $5p^5 6d$, $5p^4 6d^2$, $5p^5 7s$, $5p^4 7s^2$, $5p^5 7p$, $5p^4 7p^2$, $5p^3 6s^2 5d$, $5p^3 6s^2 4f$, $5p^3 6s^2 6p$, $5p^5 8s$, $5p7p^5$, $6p^6$ configurations for the calculation A (core [Cd], according to CC correlation) and $5p^6$, $5p^5 6s$, $5p^5 4f$, and $5p^5 5d$ configurations for the calculation B (core [Cd], according to VV correlation). These configuration sets used in calculations one can find in the supplementary material [13] denoted by A and B in Table I-VII. We reported some works related to these ion using the HFR method [2, 3]. In our previous works, we presented the energy levels, the Landé g-factors and lifetimes for $5p^6$, $5p^5 nf$ ($n = 4$, 5), $5p^5 ns$ (n = 6–8), $5p^5 np$ ($n = 6$, 7), and $5p^5 nd$ ($n = 5$, 6) excited levels [2] and $5p^6$–$5p^5 6s$, $5p^6$–$5p^5 5d$, $5p^5 6p$–$5p^5 ns$ ($n = 6$, 7), and $5p^5 6p$–$5p^5 5d$ electric dipole transitions [3] of different configuration set. In this study, we have added allowed and forbidden transitions, new energy levels, the Landé g-factors and lifetimes by two methods with configuration sets different than in [2, 3].

2. Calculation methods

We have briefly discussed HFR and MCDF methods in this study. The details of the methods have been described in [11] and [12], respectively.

In HFR method [11], for N-electron atom of nuclear charge Z_0, the Hamiltonian is expanded as

$$H = -\sum_i \nabla_i^2 - \sum_i \frac{2Z_0}{r_i} + \sum_{i>j} \frac{2}{r_{ij}} + \sum_i \zeta_i(r_i) \boldsymbol{l}_i \cdot \boldsymbol{s}_i (1)$$

in atomic units, with r_i — the distance of the i-th electron from the nucleus and $r_{ij} = |\boldsymbol{r}_i - \boldsymbol{r}_j|$. The expression $\zeta_i(R) = \frac{\alpha^2}{2} \frac{1}{r} \frac{\partial V}{\partial r}$ is the spin–orbit term, with α being the fine structure constant and V — the mean potential field due to the nucleus and other electrons. The wave function $|\rangle$ of the M sublevel of a level labeled γJ is expressed in terms of LS basis states $|\rangle$ by

$$|\gamma JM\rangle = \sum_{\alpha LS} |\alpha LSJM\rangle \langle \alpha LSJ|\gamma J\rangle . \quad (2)$$

According to HFR method, the total electric dipole (E1) transition probability from a state $\gamma' J' M'$ to all states M levels of γJ is given by

$$A_{E1} = \frac{64\pi^4 e^2 a_0^2 \sigma^3}{3h(2J'+1)} \boldsymbol{S} \quad (3)$$

and absorption oscillator strength is given by

$$f_{ij} = \frac{2(E_j - E_i)}{3(2J+1)} \boldsymbol{S}, \quad (4)$$

where $\boldsymbol{S}$ is the electric dipole line strength

$$\boldsymbol{S} = \left| \left\langle \gamma J || \boldsymbol{P}^{(1)} || \gamma' J' \right\rangle \right|^2 \quad (5)$$

in atomic units of $e^2 a_0^2$ and $\sigma = (E_j - E_i)/hc$ has units of kaysers (cm^{-1}).

The transition probability rates for pure electric quadrupole (E2) and magnetic dipole (M1) transitions are given by

$$A_{E2} = \frac{64\pi^6 e^2 a_0^4 \sigma^5}{15h(2J'+1)} \left| \left\langle \gamma J || \boldsymbol{P}^{(2)} || \gamma' J' \right\rangle \right|^2 \quad (6)$$

and

$$A_{M1} = \frac{64\pi^4 e^2 a_0^2 (\alpha/2)^2 \sigma^3}{3h(2J'+1)} \left| \left\langle \gamma J || \boldsymbol{J}^{(1)} + \boldsymbol{S}^{(1)} || \gamma' J' \right\rangle \right|^2 . \quad (7)$$

Most experiments yield the lifetime of the upper level because of easy measuring. In this case the sum over multipole transitions to all lower lying levels must be taken. The lifetime τ for a level j is defined as follows:

$$\tau_j = \frac{1}{\sum_i A_{ji}}. \quad (8)$$

In the MCDF method [12] an atomic state can be expanded as a linear combination of configuration state functions (CSFs):

$$\Psi_a(PJM) = \sum C_r(\alpha) |\gamma_r(PJM)\rangle , \quad (9)$$

where n_c is the number of CSFs included in the evaluation of atomic state functions and C_r is the mixing coefficient. The CSFs are the sum of products of single-electron Dirac spinors,

$$\phi(r, \theta, \varphi, \sigma) = \frac{1}{r} \begin{pmatrix} P(r)\chi_{\kappa m}(\theta, \varphi, \sigma) \\ iQ(r)\chi_{-\kappa m}(\theta, \varphi, \sigma) \end{pmatrix}, \quad (10)$$

where κ is a quantum number and $\chi_{\kappa m}$ is the spinor spherical harmonic in the LSJ coupling scheme and $P(r)$ and $Q(r)$ are large and small radial components of one-electron wave functions represented on a logarithmic grid.

The energy functional is based on the Dirac–Coulomb Hamiltonian in form

$$H_{\mathrm{DC}} = \sum_{j=1}^{N} \left[(c\boldsymbol{\alpha}_j \cdot \boldsymbol{p}_j) + (\beta_j - 1)c^2 + V(r_j) \right] + \sum_{j<k}^{N} \frac{1}{r_{jk}}, \quad (11)$$

where $V(r_j)$ is the electron–nucleon interaction. Once initial and final state functions have been calculated, the radiative matrix element for radiative properties computation can be obtained from

$$O_{if} = \langle \psi(i) | \boldsymbol{O}_q^{\pi(k)} | \psi(f) \rangle , \quad (12)$$

where $\boldsymbol{O}_q^{\pi(k)}$ is a spherical operator of rank k and parity π, and $\pi(\kappa)$ is $\pi = (-1)^k$, for an electric multipole transition or $\pi = (-1)^{k+1}$, for a magnetic multipole transition. The largest transition probability is for electric dipole (E1) radiation, dominated by the least factor $1/\alpha^2$ over other types of transitions (E2, M1, M2, etc.). For a transition $i \to j$, the absorption oscillator strength (f_{ij}) and transition probabilities (A_{ji}, in s^{-1}) are related by the following expression [14]:

$$f_{ij} = \frac{mc}{8\pi^2 e^2} \lambda_{ji}^2 \frac{\omega_j}{\omega_i} A_{ji} = 1.49 \times 10^{-16} \lambda_{ji}^2 \frac{\omega_j}{\omega_i} A_{ji}, \quad (13)$$

where m and e are the electron mass and charge, respectively, c is the velocity of light, λ_{ji} is the transition

energy/wavelength in Å, and ω_i and ω_j are the statistical weights of the lower i and upper j levels, respectively. Similarly, the oscillator strength f_{ij} and the line strength S (in a.u.) are related by

$$A_{ji} = \frac{2.0261 \times 10^{18}}{\omega_j \lambda_{ji}^3} S^{E1} \text{ and } f_{ij} = \frac{303.75}{\lambda_{ji} \omega_i} S^{E1}, \quad (14)$$

for the electric dipole (E1) transitions [14], and

$$A_{ji} = \frac{1.1199 \times 10^{18}}{\omega_j \lambda_{ji}^5} S^{E2} \text{ and } f_{ij} = \frac{167.89}{\lambda_{ji}^3 \omega_i} S^{E2}, \quad (15)$$

for the electric quadrupole (E2) transitions [14], and

$$A_{ji} = \frac{2.6974 \times 10^{13}}{\omega_j \lambda_{ji}^3} S^{M1} \text{ and } f_{ij} = \frac{4.044 \times 10^{-3}}{\lambda_{ji} \omega_i} S^{M1} \quad (16)$$

for the magnetic dipole (M1) transitions [14].

3. Results and discussion

We have here calculated the relativistic energies, the Landé g-factors and lifetimes for the levels of $5p^5nf$ (n = 4–10), $5p^5np$ (n = 6–10), $5p^5nh$ (n = 6–10), $5p^5nd$ (n = 5–10), $5p^5ns$ (n = 6–10), $5p^5ng$ (n = 5–10), and $5p^5ni$ (n = 7–10) configurations and the transition parameters (wavelengths, oscillator strengths, and transition probabilities) for electric dipole (E1), electric quadrupole (E2) and magnetic dipole (M1) transitions between valence excitation levels in La IV using HFR [9] and GRASP [10] codes. The selected configuration sets for investigating correlation effects have been given in Introduction. In HFR calculation, the Hamiltonian calculated eigenvalues were optimized to the observed energy levels via a least-squares fitting procedure using experimentally determined energy levels, specifically all of the levels from the NIST compilation [15]. The scaling factors of the Slater parameters (F^k and G^k) and of configuration interaction integrals (R^k), not optimized in the least-squares fitting, were chosen equal to 0.85 for calculation, while the spin–orbit parameters were left at their initial values.

The results of this work compared with available data are given in the supplementary material [13] in Tables I–VII.

In the main text comparison has been made graphically as well. The results for energy levels, the Landé g-factors and lifetimes of La IV are reported in Table II [13]. New data (energies E (cm^{-1}), the Landé g-factors, and lifetimes τ (ns)) obtained using the HFR code are given in Table I [13]. In turn, Table III [13] shows wavelengths λ (in nm and Å), logarithmic weighted oscillator strengths $\log(gf)$, and transition probabilities A_{ji} (in s^{-1}), for $5p^6$–$5p^5ns$ ($n = 6, 7, 8$), $5p^6$–$5p^5nd$ ($n = 5, 6$), $5p^5np$ ($n = 6, 7$)–$5p^5n's$ (n' = 6–8), and $5p^5np$ ($n = 6, 7$)–$5p^5n'd$ ($n' = 5, 6$) E1 transitions in La IV using HFR [9] and GRASP (E1 transitions obtained from calculation A) [10] codes. New electric dipole transitions data are given in Table IV [13]. Further, the wavelengths λ (in Å), logarithmic weighted oscillator strengths $\log(gf)$, and weighted transition probabilities A_{ji} (in s^{-1}) are reported in Table V [13], for $5p^55d$–$5p^56d$, $5p^56s$–$5p^56d$, $5p^6$–$5p^5np$ ($n = 6, 7$), $5p^56p$–$5p^57p$, $5p^5nd$–$5p^5nd$ ($n = 5, 6$), $5p^5ns$–$5p^5ns$ ($n = 6, 7$), $5p^5np$–$5p^5np$ ($n = 6, 7$), and $5p^54f$–$5p^54f$ E2 and M1 transitions (for MCDF calculation A). For E2 and M1 transitions obtained from calculation HFR, we have also prepared wavelengths λ, logarithmic weighted oscillator strengths $\log(gf)$, and weighted transition probabilities gA_{ji}, and collected them in Table VI and Table VII [13].

In presented tables [13], only odd-parity states are indicated by the superscript "^{o}". References for other comparison values are typed below the tables with a superscript lowercase letter.

3.1. Energy levels and lifetimes

The HFR and MCDF results, for relativistic energies, the Landé g-factors, and lifetimes of $5p^6$, $5p^5nf$ ($n = 4, 5$), $5p^5np$ ($n = 6, 7$), $5p^5nd$ ($n = 5, 6$), and $5p^5ns$ ($n = 6, 7, 8$) configurations in La IV are presented in the supplementary material [13] in Table II. These results have been given as energies (cm^{-1}) relative to $5p^6\ ^1S_0$ ground-state level. Except for ground-state, all levels are designated in jK-coupling and LS-coupling. The energy and lifetime of the $5p^54f$, $5p^55d$, $5p^56s$, $5p^56p$, $5p^56d$, $5p^57s$, $5p^55f$, $5p^57p$, and $5p^58s$ excited levels shown in Table II [13] have been compared with other aviable results [1, 5, 7, 8]. Importantly, these results (together with our previous work [2]) are the only results of excited levels that exist in the literature. Most of our energy results are in good agreement. In Fig. 1, we have shown the comparison between our energies and those reported by Epstein and Reader [5]. As seen from Fig. 1, the energy results obtained from our calculations are in good agreement with [5]. Linear correlation coefficient R^2 is 1.00 for calculation HFR and 0.98 for calculation MCDF.

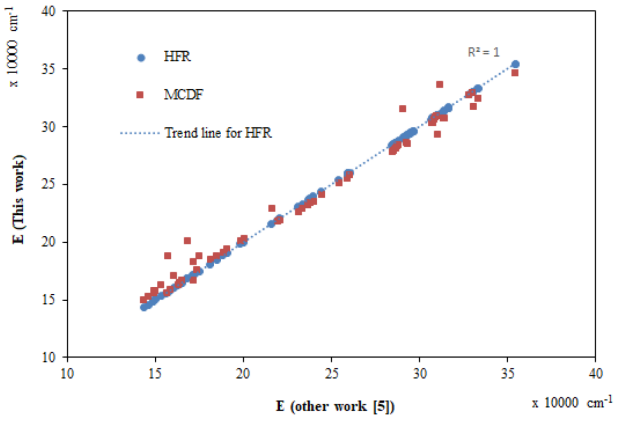

Fig. 1. Comparison of the energies obtained from this work (calculations HFR and MCDF) with those of Epstein and Reader [5].

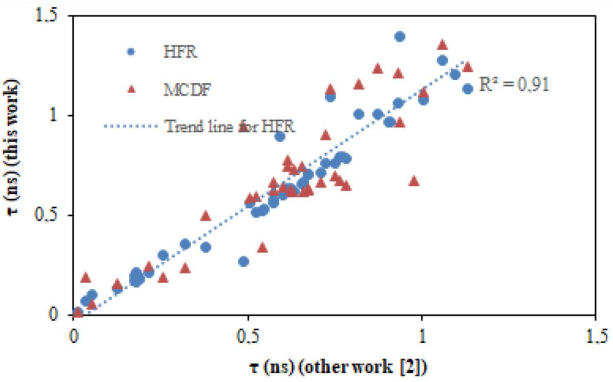

Fig. 2. Comparison of the lifetimes obtained from this work (calculations HFR and MCDF) with those of Karaçoban Usta and Şirin Yıldırım [2].

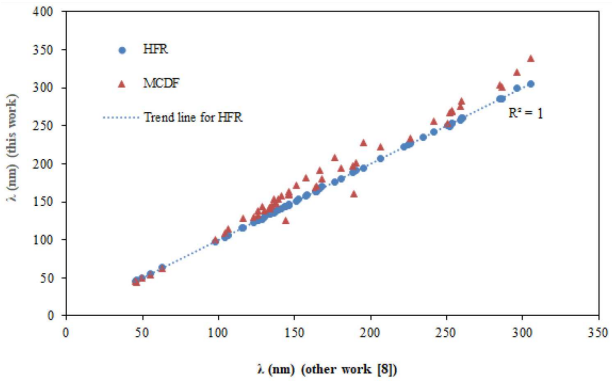

Fig. 3. Comparison of the wavelengths obtained from this work (calculations HFR and MCDF) with those of Loginov [8].

Levels of lifetimes were calculated using (8), considering all possible transitions from the listed levels to lower ones. Figure 2 shows a comparison between our lifetime results from Table II [13] and those reported by Karaçoban Usta and Şirin Yıldırım [2]. One can observe in Fig. 2 that our lifetime results are in agreement with [2], however, the lifetime values of $5p^5 5d$, $5p^5 6s\ ^3P_0^o$ and $5p^5 6s\ ^3P_2^o$ levels are not included. The coefficient of determination R^2 is 0.91 for calculation HFR. The lifetimes obtained from calculation MCDF are in agreement with other works, except $5p^5 6d\ ^1P_1^o$ and $5p^5 8s$ levels. Moreover, we have calculated the mean ratio τ(this work)/τ(other works) for the accuracy of our results. The mean ratio between our results and other works [8] have been found in the values 1.02 for calculation HFR and 0.96 for calculation MCDF. Also, we have found the values 1.07 (in calculation HFR) and 0.90 (in calculation MCDF) for the mean ratio τ(this work)/τ(other works) [2]).

The new energies, the Landé g-factors and lifetimes for $5p^5 nf$ ($n = 6$–10), $5p^5 np$ ($n = 8$–10), $5p^5 nh$ ($n = 6$–10), $5p^5 nd$ ($n = 5$–10), $5p^5 ns$ ($n = 9, 10$), $5p^5 ng$ ($n = 5$–10), and $5p^5 ni$ ($n = 7$–10) configurations are presented in Table I [13]. These data for La IV have been firstly presented in this work.

3.2. Electric dipole (E1) transitions

In the calculations HFR and MCDF, we have obtained 16 592 and 11 370 possible E1 transitions, respectively. In this work, λ (in nm), logarithmic weighted oscillator strengths $\log(gf)$, and transition probabilities A_{ji} (in s^{-1}), for $5p^6$–$5p^5 6s$, $5p^6$–$5p^5 5d$, $5p^5 6p$–$5p^5 6s$, $5p^5 6p$–$5p^5 5d$, and $5p^5 7s$–$5p^5 6p$ E1 transitions obtained using HFR [9] and GRASP [10] codes are presented in the supplementary material [13] in Table III, and compared with values reported in [1, 3, 8, 15]. We have seen a good agreement between our results with both the other works. The results are in excellent agreement with those of other work [8] for wavelengths. We have calculated the mean ratio λ(this work)/λ(other works) for the accuracy of our

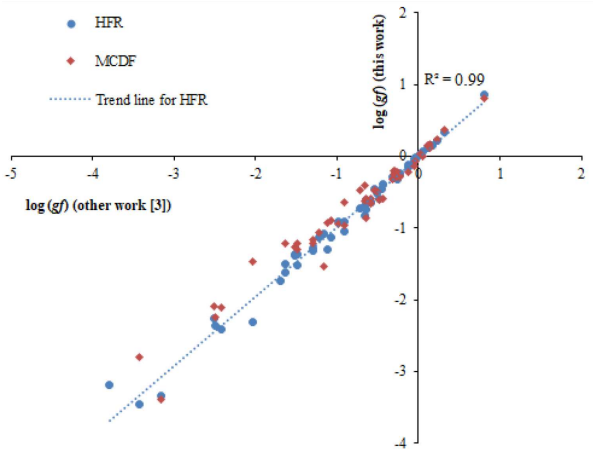

Fig. 4. Comparison of the $\log(gf)$ obtained from this work (calculations HFR and MCDF) with those of Karaçoban Usta and Şirin Yıldırım [3].

results. The mean ratio between our results and other works [8] have been found in the values 1.00 for calculation HFR and 0.99 for calculation MCDF. Additionally, the wavelengths comparison of the E1 transitions have been displayed in Fig. 3.

Comparison values of logarithmic weighted oscillator strengths results are only reported in our previous results [3]. Both HFR and MCDF results are in agreement with our previous results. We have found the values 1.01 (for HFR) and 1.04 (for MCDF) for the mean ratio of $\log(gf)$(this work)/$\log(gf)$ [3], except the transition 125.91 nm (for MCDF) and also compared graphically (in Fig. 4). The transition probability results given in Table III [13] are compared with the results reported by Loginov [8]. For some transitions, although the agreement is less with the Loginov results, it is good with our previous work [3]. Except the transitions 222.225, 135.228, 126.071, 195.259, 164.553 nm (HFR and MCDF calculations), 126.071 nm (HFR calculation), 180.736, and 189.147 nm (MCDF calculation), we have found the

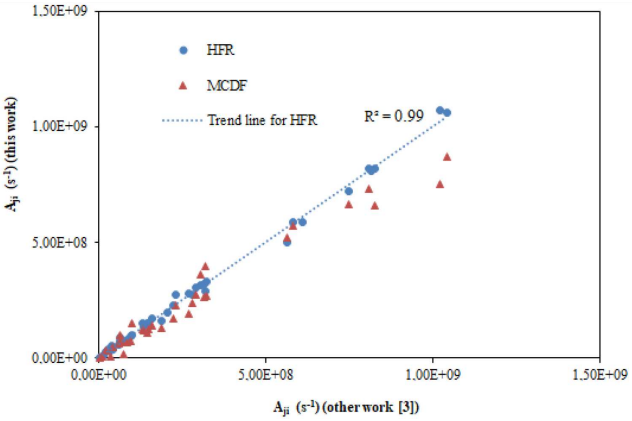

Fig. 5. Comparison of the transition probabilities obtained from this work (calculations HFR and MCDF) with those of Karaçoban Usta and Şirin Yıldırım [3].

values 1.020 and 0.990 for the mean ratio of A_{ji}(this work)/A_{ji} [8], respectively. Also, the transition probability comparison of the E1 transitions have been displayed in Fig. 5. It is comparison of the transition probabilities obtained from this work with those of Karaçoban Usta and Şirin Yıldırım [3].

We have also reported new wavelengths λ (Å), logarithmic weighted oscillator strengths $\log(gf)$, and transition probabilities A_{ji} (s^{-1}) for atomic data. In the supplementary material [13], Table IV shows $5p^5ns$ $(n = 7, 8)$–$5p^6$, $5p^56d$–$5p^6$, $5p^5np$ $(n = 6, 7)$–$5p^5n'd$ $(n' = 5, 6)$, and $5p^5np$ $(n = 6, 7)$–$5p^5n's$ $(n' = 6, 7, 8)$ E1 transitions obtained from calculations HFR and MCDF. These data for La IV are presented for the first time.

3.3. Forbidden transitions

Observations of weak or forbidden transition lines have become possible with increasing efficiency of experimental techniques. These transitions are of great importance in the astrophysical fields. To date, there is no theoretical or experimental study on the forbidden transition parameters for La IV. In this work, the data on forbidden (electric quadrupole (E2) and magnetic dipole (M1)) transitions for this ion have been firstly presented using calculations HFR and MCDF. It has been obtained as 24 883 for E2 and 16 394 for M1 transitions in HFR calculation and 29 468 for E2 and 21 542 for M1 transitions in MCDF calculation.

The wavelengths λ (in Å), logarithmic weighted oscillator strengths $\log(gf)$, and weighted transition probabilities A_{ji} (in s^{-1}), for $5p^55d$–$5p^56d$, $5p^56s$–$5p^56d$, $5p^6$–$5p^5np$ $(n = 6, 7)$, $5p^56p$–$5p^57p$, $5p^5nd$–$5p^5nd$ $(n = 5, 6)$, $5p^5ns$–$5p^5ns$ $(n = 6, 7)$, $5p^5np$–$5p^5np$ $(n = 6, 7)$, and $5p^54f$–$5p^54f$ E2 and M1 transitions (for MCDF calculation A) have been given in Table V (see [13]). All values obtained from the HFR and MCDF calculations are in agreement with each other. Some small difference has arisen from the fact that both methods involved different contributions. Also, for new data shown in Table VI and VII (see [13]), we have reported wavelengths λ, logarithmic weighted oscillator strengths $\log(gf)$, and weighted transition probabilities gA_{ji}. These weighted transition probabilities are greater than or equal to 10^4 for E2 transitions and 10^2 for M1 transitions for calculation HFR.

4. Conclusion

The main purpose of this paper is to perform the HFR and MCDF calculations to obtain a description of the La IV spectrum. New energies, the Landé g-factors, and lifetimes for excited levels, and E1, E2 and M1 transitions are reported in Tables I–VII, in the supplementary material [13]. Further, including other our results obtained from this work can be obtained from corresponding author. E2 and M1 transitions of La IV have been obtained for the first time for transitions between excited states. Our calculations have been compared to other works, and good agreements have been obtained from the comparisons. Hopefully, data in this paper will facilitate experimental studies.

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