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Research Article

Energy Levels and the Landé g-Factors for Singly Ionized Lanthanum

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We have calculated the energies and the Landé g-factors for $5d^2$, 5d6s, $6s^2$, 4f6p, 5d7s, 5d6d, $4f^2$, $6p^2$, 6s6d, 6s7s, 4f6s, 4f5d, 5d6p, 6s6p, 4f7s, 4f6d, 5d7p, and 6s7p excited levels of singly ionized lanthanum (La II). These calculations have been carried out by using the multiconfiguration Hartree-Fock method within the framework of the Breit-Pauli Hamiltonian (MCHF+BP) and the relativistic Hartree-Fock (HFR) method. The obtained results have been compared with other works available in the literature. A discussion of these calculations for La II in this study has also been in view of the MCHF+BP and HFR methods.

1. Introduction

Lanthanides constitute a group of elements characterized by similar chemical and physical properties. The presence of this group in the periodic table is determined by behaviour of the radial part of the wave function for the 4f orbital, which collapses for the values of atomic number $Z > 57$ and fills in the first (internal) minimum of the electrostatic potential [1]. The rare-earth element lanthanum ($Z = 57$) is a product of neutron-capture fusion reactions that occur in the late stages of stellar evolution. Lanthanum's abundance relative to other rare earths in stars of different metallicities can lead to insights on the nature of the dominant neutron-capture production sites throughout the Galaxy's history [2].

The lanthanum atom is the first member of the rare-earth elements. It has two naturally occurring isotopes: ^{138}La (0.085%) and ^{139}La (99.910%). Meggers viewed first the spectra of singly ionized lanthanum [3, 4]. Later, Russell and Meggers analyzed the spectra of La II [5]. Grevesse and Blanquet determined the abundance of singly ionized lanthanum in the sun [6]. Spector and Gotthelf performed configuration interaction in La II [7]. Xie and coworkers investigated Rydberg and autoionization states of the singly ionized lanthanum [8]. First, ionization potential of lanthanides by laser spectroscopy was studied by Worden et al. [9]. Sugar and Reader obtained by means of a semiempirical calculation ionization potential of singly ionized lanthanum [10]. Eliav et al. reported ionization potential and excitation energies of La II [11]. Theoretical energy levels in La II were calculated by Kułaga-Egger and Migdałek [12]. In the past, different groups [13–26] investigated oscillator strengths, transition probabilities, lifetimes, and the hyperfine structure in singly ionized lanthanum by various experimental and theoretical methods. A list of energy levels for excited states was completed and presented by Sansonetti and Martin [27] and can be found on the NIST website [28].

In this work, we have presented the energies and the Landé g-factors for $5d^2$, 5d6s, $6s^2$, 4f6p, 5d7s, 5d6d, $4f^2$, $6p^2$, 6s6d, 6s7s, 4f6s, 4f5d, 5d6p, 6s6p, 4f7s, 4f6d, 5d7p, and 6s7p excited levels of singly ionized lanthanum (La II). Calculations have been carried out by the multiconfiguration Hartree-Fock method within the framework of the Breit-Pauli Hamiltonian (MCHF+BP) [29] and the relativistic Hartree-Fock (HFR) method [30]. These codes consider the correlation effects and relativistic corrections. These effects make an important contribution to understanding physical and chemical properties of atoms or ions, especially lanthanides. The ground-state configuration of La II is [Xe] $5d^2\ ^3F_2$. We took into account with various configuration sets according to valence-valence and core-valence correlations for correlation effects outside the core [Xe] in La II. These configuration sets used in calculations have been

Table 1: Configuration sets taken for La II in MCHF+BP and HFR calculations.

Levels	Configurations			
	A	B	C	D
	For MCHF+BP calculations			
Even-parity	nd^2 (n = 5, 6), $4f^2$, 5d6d, 6s6d, 4fnp, 5dns, ns^2, np^2 (n = 6–9), 6sns, 6pnp, 6dns (n = 7–9), 7sns, 7pnp (n = 8, 9), 8s9s, 8p9p	As in calculation A	$5p^65d^2$, $5p^65d6s$, $5p^66s^2$, $5p^64f6p$, $5p^64f^2$, $5p^54f6s^2$, $5p^55d^26p$, $5p^56s^26p$	$5p^6nd^2$ (n = 5, 6), $5p^64f^2$, $5p^65d6d$, $5p^66s6d$, $5p^64fnp$, $5p^65dns$, $5p^6ns^2$, $5p^6np^2$ (n = 6–9), $5p^66sns$, $5p^66dns$, $5p^66pnp$ (n = 7–9), $5p^67sns$ (n = 8, 9), $5p^67p8p$, $5p^68s9s$, $5p^68p9p$
Odd-parity	4f6s, 4f5d, 5dnp, 6snp (n = 6–9), 6pns, 7snp (n = 7–9), 7pns, 8snp (n = 8, 9), 8p9s, 9s9p	As in calculation A	$5p^64f6s$, $5p^64f5d$, $5p^65d6p$, $5p^54f^26s$, $5p^55d6s^2$, $5p^55d6p^2$	
	For HFR calculations			
Even-parity	$5d^2$, 5d6s, $6s^2$, 4f6p, $4f^2$	$5d^2$, 5d6s, $6s^2$, 4f6p, 5d7s, 5d6d, $4f^2$, $6p^2$, 6s6d, 6s7s		
Odd-parity	4f6s, 4f5d, 5d6p, 6s6p	4f6s, 4f5d, 5d6p, 6s6p, 4f7s, 4f6d, 5d7p, 6s7p		

denoted by A, B, C, and D for the MCHF+BP, and A and B for the HFR calculations and given in Table 1. We have performed the atomic structure calculations on lanthanide atoms and ions, systematically. We reported some works related to these atoms and ions using the methods mentioned above [31–42]. In addition, we presented the energies of $5d^2$, 5d6s, $6s^2$, and $6p^2$ excited levels and ionization energy for La II by the MCHF+BP method [34]. In this work, we have considered more levels than in [34] and added the Landé g-factors for these levels.

2. Calculation Methods: MCHF and HFR

In the MCHF method [29], atomic state functions can be obtained as a linear combination of configuration state functions (CSFs) in LS coupling,

$$\Psi(\gamma LS) = \sum_{i=1}^{M} c_i \Phi(\gamma_i LS), \qquad \sum_{i=1}^{M} c_i^2 = 1. \tag{1}$$

The mixing coefficients $\{c_i\}$ and the radial orbitals are optimized simultaneously, based on the expectation values $\langle\Psi|H|\Psi\rangle$.

In the MCHF method, the Breit-Pauli Hamiltonian for relativistic corrections is taken as a perturbation with order α^2. The Breit-Pauli Hamiltonian includes relativistic effects. This Hamiltonian can be written as follows:

$$H_{\mathrm{BP}} = H_{\mathrm{NR}} + H_{\mathrm{RS}} + H_{\mathrm{FS}}, \tag{2}$$

where H_{NR} is the nonrelativistic many-electron Hamiltonian and H_{RS} is the relativistic shift operator including mass correction, one- and two-body Darwin terms, spin-spin contact term, and orbit-orbit term; fine structure Hamiltonian H_{FS} consists of the spin-orbit, spin-other-orbit, and spin-spin terms. Now, the multiconfiguration wave functions are obtained as linear combinations of CSFs in LSJ coupling. Therefore, the radial functions building the CSFs are taken from a previous nonrelativistic MCHF run and only the expansion coefficients are optimized. Therefore, the matrix eigenvalue problem becomes

$$\mathbf{H}c = Ec, \tag{3}$$

where $\mathbf{H}$ is the Hamiltonian matrix with the following elements

$$H_{ij} = \left\langle \gamma_i L_i S_i JM \left| H_{\mathrm{BP}} \right| \gamma_j L_j S_j JM \right\rangle. \tag{4}$$

The Breit-Pauli Hamiltonian is a first order perturbation correction to the nonrelativistic Hamiltonian. The Landé g-factor of an atomic level is related to the energy shift of the sublevels having magnetic number M by

$$\Delta E(\gamma LS) = \mu_B B g_{\gamma J} M, \tag{5}$$

where B is the magnetic field intensity and μ_B is the Bohr magneton. In pure LS coupling, the Landé g-factor can be taken given by formula (8) in [43]. The Landé g-factors for energy levels are a valuable aid in the analysis of a spectrum. These factors which are a measure of the magnetic sensitivity of atomic levels can be calculated using the code developed by Jönsson and Gustafsson [43] according to MCHF wave functions.

In the HFR method [30], for N electron atom of nuclear charge Z_0, the Hamiltonian is expanded as

$$\mathbf{H} = -\sum_i \nabla_i^2 - \sum_i \frac{2Z_0}{r_i} + \sum_{i>j} \frac{2}{r_{ij}} + \sum_i \zeta_i(r_i)\, \mathbf{l}_i \cdot \mathbf{s}_i \tag{6}$$

in atomic units with the distance r_i of the ith electron from the nucleus and $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$. $\zeta_i(R) = (\alpha^2/2)(1/r)(\partial V/\partial r)$ is the spin-orbit term with α the fine structure constant and V the mean potential field due to the nucleus and other electrons.

Wave function $|\gamma JM\rangle$ of the M sublevel of a level labeled γJ is expressed in terms of LS basis states $|\alpha LSJM\rangle$ by the following formula:

$$|\gamma JM\rangle = \sum_{\alpha LS} |\alpha LSJM\rangle \langle \alpha LSJ \mid \gamma J\rangle . \quad (7)$$

Using determinant wave functions for the atom, total binding energy is given by

$$E = \sum_i \left(E_k^i + E_n^i + \sum_{j<i} E^{ij} \right), \quad (8)$$

where E_k^i is the kinetic energy, E_n^i is the electron-nuclear energy, and E_{ij} is the Coulomb interaction energy between electron i and j, averaged over all possible magnetic quantum numbers.

This method calculates one-electron radial wave functions for each of any number of specified electron configurations, using the Hartree-Fock or any of several more approximate methods. It obtains the center-of-gravity energy of each configuration and those radial Coulomb and spin-orbit integrals required to calculate the energy levels for the configuration. After the wave functions have been obtained, they are used to calculate the configuration-interaction Coulomb integrals between each pair of interacting configurations. Then, energy matrices are set up for each possible value of J, and each matrix is diagonalized to get eigenvalues (energy levels) and eigenvectors (multiconfiguration, intermediate coupling wave functions in various possible angular-momentum coupling representations).

Relativistic corrections to total binding energies become quite large for heavy elements; the main contributions come from the tightly bound inner electrons. In the HFR method there have been limited calculations to the mass-velocity and Darwin corrections by using relativistic correction to total binding energy:

$$E_r = \sum_i E_r^i = \sum_i \left(E_m^i + E_D^i \right). \quad (9)$$

The Landé g-factors in HFR calculations have the same formula as in MCHF calculations. Here, the calculations for the Landé g-factors have been performed according to HFR wave functions.

3. Results and Discussion

Here, we have calculated the energies and the Landé g-factors for $5d^2$, 5d6s, $6s^2$, 4f6p, 5d7s, 5d6d, $4f^2$, $6p^2$, 6s6d, 6s7s, 4f6s, 4f5d, 5d6p, 6s6p, 4f7s, 4f6d, 5d7p, and 6s7p excited levels outside the core [Xe] in La II using the MCHF+BP [44] and HFR [45] codes. We have presented the several excited level energies and transition energies for La I and La II [34]. We have performed new various calculations for obtaining configuration state functions (CSFs) according to valence-valence and core-valence correlations. Moreover, it is well known that the Landé g-factors are important in many scientific areas such as astrophysics. Table 1 displays the various configuration sets for considering correlation effects. The results for energy levels and the Landé g-factors of La II have been reported in Table 2. In this table, the calculations for the various configuration sets are represented by A, B, C, and D for the MCHF+BP and by A and B for the HFR calculations. A comparison is also made with other calculations and experiments in the table. References for other comparison values are typed below the table with a superscript lowercase letter. Only odd-parity states in table are indicated by the superscript "o."

Electron correlation effects and relativistic effects play an important role in the spectra of heavy elements. Thus, we have to consider these effects for lanthanides. However, it is very difficult to calculate the electron correlation for these atoms because of their complex structures. Although this provides useful information for understanding the correlation effect, computer constraints occur. Therefore, we increasingly varied some parameters in the MCHF atomic structure package (maximum number of eigenpairs, maximum number of configuration state functions, maximum number of terms, and maximum number of coefficients) so that the calculations for the configurations above could reasonably be made. The energies and the Landé g-factors for $5d^2$, 5d6s, $6s^2$, 4f6p, 5d7s, 5d6d, $4f^2$, $6p^2$, 6s6d, 6s7s, 4f6s, 4f5d, 5d6p, 6s6p, 4f7s, 4f6d, 5d7p, and 6s7p excited levels outside the core [Xe] in La II are calculated by the MCHF+BP and HFR methods. The obtained results have been presented as energies (cm^{-1}) relative to $5d^2\ {}^3F_2$ ground state in Table 2.

In the MCHF+BP calculations, it is taken into account core [Xe] for calculations A and B and core [Cd] for calculations C and D for La II. The odd- and even-parity levels of calculations A, B, and D are considered the only interaction between the valence electrons, whereas odd- and even-parity levels of calculation C were an included interaction between valence-valence electrons and core-valence electrons. In the MCHF+BP method, firstly, for configurations selected according to valence-valence and core-valence correlations, the non-relativistic wave functions and energies were obtained. In the configuration interaction method, energy levels are performed using wave functions obtained taking into account relativistic corrections. Then the Landé g-factors for energy levels are calculated using the Zeeman program developed by Jönsson and Gustafsson [43].

In the MCHF+BP calculations, we have reported that the levels belong to $5d^2$, 5d6s, $6s^2$, 5d6d, $6p^2$, and 6s6d for even-parity and 4f6s, 4f5d, 5d6p, and 6s6p for odd-parity in Table 2. We presented the energies of several even-parity levels from obtained calculation A in [34]. Although configurations of calculation B are the same with calculations of calculation A, MCHF run is different. When our MCHF+BP results were compared with others [12, 28], the energies for most of levels are in agreement. $5d^2\ {}^3F$ levels obtained from calculations A and D and $5d^2\ {}^3P$ levels obtained from calculations A and C are good in agreement with other works. The agreement is

Table 2: Energies, E, and the Landé g-factors for some levels in La II.

Levels		E (cm^{-1})			g-Factors		
		This work			This work		
Conf.	Term	MCHF+BP	HFR	Other works	MCHF+BP	HFR	Other works
			For even-parity				
$5d^2$	$^3F_2$	0.00[A,B,C,D]	−0.13[A]	0.00[a]	0.728[A]	0.732[A]	0.721[a]
			0.02[B]	−4[b]	0.709[B]	0.736[B]	
					0.715[C]		
					0.722[D]		
	$^3F_3$	1100.72[A]	1018.92[A]	1016.100[a]	1.083[A,B,C,D]	1.084[A,B]	1.038[a]
		816.18[B]	1046.86[B]	1028[b]			
		743.03[C]					
		898.90[D]					
	$^3F_4$	2131.38[A]	1935.49[A]	1970.700[a]	1.249[A,B,C]	1.249[A,B]	1.248[a]
		1612.45[B]	1974.01[B]	1963[b]	1.250[D]		
		1456.54[C]					
		1741.31[D]					
$5d^2$	$^1D_2$	1379.80[A]	1394.91[A]	1394.460[a]	0.993[A]	0.965[A]	0.977[a]
		1443.25[B]	1393.79[B]	1395[b]	0.968[B,C]	0.959[B]	
		1236.03[C]			0.955[D]		
		1398.12[D]					
$5d^2$	$^3P_0$	5377.78[A]	5228.71[A]	5249.700[a]			
		5918.77[B]	5265.77[B]	5244[b]			
		5575.39[C]					
		5654.01[D]					
	$^3P_1$	6000.10[A]	5769.81[A]	5718.120[a]	1.501[A,B,C,D]	1.501[A,B]	1.497[a]
		6374.80[B]	5737.42[B]	5725[b]			
		5867.74[C]					
		6132.57[D]					
	$^3P_2$	6513.01[A]	6261.60[A]	6227.420[a]	1.485[A]	1.489[A]	1.481[a]
		6798.78[B]	6239.70[B]	6224[b]	1.494[B,D]	1.488[B]	
		6247.36[C]			1.497[C]		
		6588.07[D]					
$5d^2$	$^1G_4$	8739.05[A]	7445.09[A]	7473.320[a]	1.002[A]	1.002[A,B]	1.000[a]
		8468.71[B]	7374.70[B]	7476[b]	1.001[B,C,D]		
		8941.04[C]					
		9027.98[D]					
$5d^2$	$^1S_0$	16629.75[A]	16453.30[A]	—			
		18979.63[B]	13675.30[B]				
		18143.98[D]					
5d6s	$^3D_1$	1662.59[A]	1893.01[A]	1895.150[a]	0.499[A,B,C,D]	0.499[A,B]	0.498[a]
		2481.69[B]	1898.19[B]	1902[b]			
		1994.95[C]					
		2533.26[D]					
	$^3D_2$	2476.73[A]	2580.06[A]	2591.600[a]	1.119[A]	1.143[A]	1.133[a]
		2939.18[B]	2549.72[B]	2572[b]	1.159[B]	1.144[B]	
		2550.88[C]			1.154[C]		
		3010.41[D]			1.160[D]		
	$^3D_3$	3094.79[A]	3311.82[A]	3250.350[a]	1.334[A,B,C,D]	1.334[A,B]	1.334[a]
		3501.39[B]	3255.89[B]	3260[b]			
		3204.83[C]					
		3614.27[D]					
5d6s	$^1D_2$	10064.87[A]	10088.91[A]	10094.800[a]?	1.010[A]	1.006[A,B]	1.005[a]

Table 2: Continued.

Levels		E (cm^{-1})			g-Factors		
Conf.	Term	This work		Other works	This work		Other works
		MCHF+BP	HFR		MCHF+BP	HFR	
		11480.98[B]	10095.00[B]	10096[b]	1.003[B,D]		
		13078.05[C]			1.001[C]		
		11980.57[D]					
$6s^2$	$^1S_0$	6428.50[A]	7371.89[A]	7394.570[a]			
		6664.52[B]	7393.30[B]	7395[b]			
		9713.71[C]					
		6709.28[D]					
4f6p	$^3F_2$	—	35544.74[A]	35787.53[a]	—	0.669[A]	0.719[a]
			35756.53[B]	35771[b]		0.747[B]	
	$^3F_3$	—	35687.88[A]	36954.65[a]	—	1.050[A]	1.061[a]
			37062.30[B]	36953[b]		1.005[B]	
	$^3F_4$	—	37018.59[A]	37790.57[a]	—	1.212[A]	1.113[a]
			37733.47[B]	37779[b]		1.105[B]	
4f6p	$^1F_3$	—	36917.97[A]	37209.71[a]	—	0.934[A]	0.944[a]
			37302.79[B]	37243[b]		1.036[B]	
4f6p	$^3G_3$	—	37604.82[A]	35452.66[a]	—	0.854[A]	0.876[a]
			35373.81[B]	35465[b]		0.856[B]	
	$^3G_4$	—	37768.59[A]	37172.79[a]	—	1.068[A]	1.127[a]
			37186.27[B]	37157[b]		1.098[B]	
	$^3G_5$	—	39201.02[A]	39018.74[a]	—	1.200[A,B]	1.21[a]
			39035.52[B]	39007[b]			
4f6p	$^3D_1$	—	38123.37[A]	38534.11[a]	—	0.499[A,B]	0.497[a]
			38536.02[B]	38545[b]			
	$^3D_2$	—	38214.22[A]	38221.49[a]	—	1.131[A]	1.071[a]
			38070.87[B]	38210[b]		1.027[B]	
	$^3D_3$	—	39512.21[A]	39402.55[a]	—	1.329[A]	1.274[a]
			39535.50[B]	39403[b]		1.270[B]	
4f6p	$^1G_4$	—	38968.77[A]	39221.65[a]	—	1.021[A]	1.059[a]
			39162.52[B]	39235[b]		1.097[B]	
4f6p	$^1D_2$	—	40343.10[A]	40457.71[a]	—	1.033[A]	1.036[a]
			40233.91[B]	40456[b]		1.059[B]	
5d7s	$^3D_1$	—	49703.78[B]	49733.13[a]	—	0.500[B]	0.500[a]
				49714[b]			
	$^3D_2$	—	49952.52[B]	49884.35[a]	—	1.128[B]	1.117[a]
				49905[b]			
	$^3D_3$	—	51238.10[B]	51228.57[a]	—	1.307[B]	1.315[a]
				51235[b]			
5d7s	$^1D_2$	—	51501.10[B]	51523.86[a]	—	1.058[B]	1.036[a]
				51516[b]			
5d6d	$^1F_3$	70728.01[A]	51978.02[B]	52137.67[a]	0.978[A]	1.048[B]	0.987[a]
		74919.76[B]		52216[b]	1.056[B]		
5d6d	$^3D_1$	71108.98[A]	52220.02[B]	52169.66[a]	0.544[A]	0.557[B]	0.621[a]
		75022.05[B]		52148[b]	0.622[B]		
	$^3D_2$	71922.34[A]	52746.60[B]	52734.81[a]	1.167[A]	1.126[B]	1.154[a]
		75364.62[B]		52728[b]	1.033[B]		
	$^3D_3$	72905.11[A]	53276.41[B]	53689.56[a]	1.302[A]	1.297[B]	1.218[a]
		75927.05[B]		53647[b]	1.119[B]		
5d6d	$^1P_1$	74454.96[A]	53356.36[B]	53302.56[a]	1.048[A]	1.343[B]	1.335[a]

Table 2: Continued.

Levels		E (cm^{-1})			g-Factors		
		This work			This work		
Conf.	Term	MCHF+BP	HFR	Other works	MCHF+BP	HFR	Other works
		75644.43[B]		53317[b]	1.373[B]		
5d6d	$^3F_2$	86857.66[A]	53855.01[B]	53885.24[a]	0.687[A]	0.741[B]	0.751[a]
		75086.62[B]		53914[b]	0.847[B]		
	$^3F_3$	76042.84[B]	54392.59[B]	54840.04[a]	1.161[B]	1.050[B]	1.088[a]
				54755[b]			
	$^3F_4$	88422.30[A]	54664.69[B]	55321.35[a]	1.196[A]	1.139[B]	1.136[a]
		76155.48[B]		55303[b]	1.212[B]		
5d6d	$^3S_1$	—	54175.01[B]	54365.80[a]	—	1.566[B]	1.455[a]
				54370[b]			
5d6d	$^1S_0$	74225.09[B]	54244.49[B]	54793.82[a]			
5d6d	$^1D_2$	84447.02[A]	55024.06[B]	55184.05[a]	0.996[A]	1.056[B]	1.183[a]
		76453.25[B]		55208[b]	1.051[B]		
5d6d	$^3G_3$	69310.22[A]	55169.13[B]	52857.88[a]	0.803[A]	0.798[B]	0.861[a]
		75153.22[B]		52878[b]	0.831[B]		
	$^3G_4$	70592.95[A]	55607.00[B]	53333.37[a]	1.050[A]	1.069[B]	1.036[a]
		75339.70[B]		53368[b]	1.070[B]		
	$^3G_5$	71830.19[A]	56214.97[B]	54434.65[a]	1.200[A,B]	1.200[B]	1.21[a]
		76224.45[B]		54435[b]			
5d6d	$^3P_0$	90419.13[A]	55630.81[B]	54964.19[a]			
		76456.13[B]		54786[b]			
	$^3P_1$	90863.55[A]	55411.73[B]	55230.33[a]	1.501[A]	1.535[B]	1.552[a]
		76858.62[B]		55352[b]	1.626[B]		
	$^3P_2$	91525.97[A]	55746.81[B]	56036.60[a]	1.488[A]	1.392[B]	1.203[a]
		76983.87[B]		56090[b]	1.385[B]		
5d6d	$^1G_4$	76564.89[B]	59068.02[B]	56035.70[a]	1.018[B]	1.056[B]	1.027[a]
				55076[b]			
$4f^2$	$^3H_4$	—	55201.97[A]	55107.25[a]	—	0.839[A]	0.883[a]
			53676.92[B]	55079[b]		0.887[B]	
	$^3H_5$	—	56092.25[A]	55982.09[a]	—	1.033[A,B]	1.033[a]
			55318.80[B]	55995[b]			
	$^3H_6$	—	56863.10[A]	56837.94[a]	—	1.166[A]	1.14[a]
			56547.89[B]	59845[b]		1.165[B]	
$4f^2$	$^1G_4$	—	56394.91[A]	59527.60[a]	—	0.974[A]	1.046[a]
			55328.98[B]	59522[b]		1.016[B]	
$4f^2$	$^3F_2$	—	57396.38[A]	57399.58[a]	—	0.672[A]	0.675[a]
			56706.59[B]	57385[b]		0.680[B]	
	$^3F_3$	—	57884.41[A]	57918.50[a]	—	1.084[A]	1.085[a]
			57513.31[B]	57936[b]		1.083[B]	
	$^3F_4$	—	58533.37[A]	58259.41[a]	—	1.237[A]	1.196[a]
			58315.69[B]	58264[b]		1.184[B]	
$4f^2$	$^1I_6$	—	61521.93[A]	62408.40[a]	—	1.001[A]	1.003[a]
			61759.71[B]			1.002[B]	
$4f^2$	$^1D_2$	—	62065.79[A]	62026.27[a]	—	1.028[A]	1.054[a]
			62417.80[B]	62029[b]		1.044[B]	
$4f^2$	$^3P_0$	—	63593.22[A]	63463.95[a]	—		
			64001.07[B]	63496[b]			
	$^3P_1$	—	63865.10[A]	63703.18[a]	—	1.501[A,B]	1.471[a]
			64480.52[B]	63736[b]			

Table 2: Continued.

Levels		E (cm^{-1})			g-Factors		
		This work			This work		
Conf.	Term	MCHF+BP	HFR	Other works	MCHF+BP	HFR	Other works
	$^3P_2$	—	64283.97[A]	64278.92[a]	—	1.467[A]	1.414[a]
			65194.71[B]	64214[b]		1.449[B]	
$4f^2$	$^1S_0$	—	69782.30[A]	69505.06[a]	—		
			71321.50[B]				
$6p^2$	$^1D_2$	61118.75[A]	59830.40[B]	59900.08[a]	1.205[A]	1.061[B]	1.035[a]
		63903.98[B]		59899[b]	1.013[B]		
		68314.29[D]			1.005[D]		
$6p^2$	$^3P_0$	57741.75[A]	60001.21[B]	60094.84[a]			
		57033.69[B]		60091[b]			
		58691.43[D]					
	$^3P_1$	58647.09[A]	60514.89[B]	61128.83[a]	1.501[A,B,D]	1.502[B]	1.528[a]
		57752.71[B]		61132[b]			
		59347.37[D]					
	$^3P_2$	59269.90[A]	61418.50[B]	62506.36[a]	1.296[A]	1.435[B]	1.416[a]
		58826.49[B]		62504[b]	1.488[B]		
		60398.00[D]			1.496[D]		
$6p^2$	$^1S_0$	70729.58[A]	66977.30[B]	66591.91[a]			
		83062.12[B]					
		82414.06[D]					
6s6d	$^3D_1$	79297.74[A]	63251.92[B]	64361.28[a]	0.499[A.B]	0.499[B]	0.506[a]
		86162.37[B]		64374[b]			
	$^3D_2$	79538.63[A]	63833.97[B]	64529.90[a]	1.133[A]	1.165[B]	1.217[a]
		86172.16[B]		64509[b]	1.166[B]		
	$^3D_3$	80684.92[A]	64853.61[B]	64692.59[a]	1.334[A.B]	1.334[B]	—
		86191.20[B]		64701[b]			
6s6d	$^1D_2$	86532.15[B]	69906.50[B]	—	1.001[B]	1.003[B]	—
6s7s	$^3S_1$	—	61127.80[B]	60660.18[a]?	—	2.001[B]	1.955[a]
				60660[b]			
6s7s	$^1S_0$	—	63307.50[B]				
For odd-parity							
4f6s	$^3F^o_2$	14378.61[A]	14174.39[A]	14147.980[a]	0.666[A,C]	0.666[A,B]	0.664[a]
		14264.12[B]	14267.68[B]	14184[b]	0.669[B]		
		13925.11[C]					
	$^3F^o_3$	14756.50[A]	14283.31[A]	14375.170[a]	1.060[A,C]	1.055[A]	1.056[a]
		14858.62[B]	14256.22[B]	14338[b]	1.068[B]	1.047[B]	
		14291.70[C]					
	$^3F^o_4$	16270.43[A]	15651.91[A]	15698.740[a]	1.250[A,B]	1.250[A]	1.247[a]
		16250.88[B]	15747.51[B]	15682[b]	1.251[C]	1.245[B]	
		15785.08[C]					
4f6s	$^1F^o_3$	16349.78[A]	15822.29[A]	15773.770[a]	1.023[A,C]	1.028[A]	1.017[a]
		16448.12[B]	15725.69[B]	15790[b]	1.016[B]	1.037[B]	
		15889.78[C]					
4f5d	$^1G^o_4$	23958.81[A]	16965.67[A]	16559.170[a]	0.971[A,C]	0.905[A]	0.969[a]
		25542.89[B]	15525.19[B]	16630[b]	1.059[B]	1.005[B]	
		23797.47[C]					
4f5d	$^3F^o_2$	25007.46[A]	17448.60[A]	17211.930[a]	0.725[A]	0.713[A]	0.754[a]
		28148.54[B]	18658.83[B]	17196[b]	0.685[B]	0.680[B]	
		24733.62[C]			0.735[C]		

Table 2: Continued.

Levels		E (cm^{-1})			g-Factors		
		This work			This work		
Conf.	Term	MCHF+BP	HFR	Other works	MCHF+BP	HFR	Other works
	$^3F^o_3$	25740.72[A]	18242.30[A]	18235.560[a]	1.091[A]	1.083[A]	1.086[a]
		29158.71[B]	18866.08[B]	18215[b]	1.083[B]	1.079[B]	
		25479.83[C]			1.098[C]		
	$^3F^o_4$	27201.89[A]	19267.37[A]	19214.540[a]	1.225[A]	1.226[A]	1.232[a]
		30358.80[B]	19233.10[B]	19199[b]	1.241[B]	1.241[B]	
		26932.00[C]			1.224[C]		
4f5d	$^3H^o_4$	25669.19[A]	17727.74[A]	17825.620[a]	0.855[A]	0.920[A]	0.846[a]
		27280.97[B]	17683.40[B]	17803[b]	0.862[B]	0.806[B]	
		25499.67[C]			0.856[C]		
	$^3H^o_5$	26756.81[A]	18250.23[A]	18580.410[a]	1.033[A,B,C]	1.034[A,B]	1.017[a]
		28223.06[B]	18122.03[B]	18573[b]			
		26582.89[C]					
	$^3H^o_6$	28460.49[A]	19394.18[A]	19749.620[a]	1.167[A,C]	1.167[A,B]	1.178[a]
		28275.22[C]	18802.98[B]	19767[b]			
4f5d	$^1D^o_2$	31071.25[A]	19151.58[A]	18895.410[a]	0.981[A]	0.970[A]	0.923[a]
		32636.97[B]	21057.91[B]	18926[b]	0.997[B]	1.114[B]	
		30916.96[C]			0.982[C]		
4f5d	$^3G^o_3$	31665.41[A]	20315.59[A]	20402.820[a]	0.763[A]	0.757[A]	0.757[a]
		34021.44[B]	21064.80[B]	20405[b]	0.758[B]	0.782[B]	
		31554.09[C]			0.764[C]		
	$^3G^o_4$	32976.84[A]	21247.80[A]	21331.600[a]	1.050[A,B,C]	1.049[A]	1.049[a]
		35195.62[B]	21629.90[B]	21324[b]		1.054[B]	
		32859.39[C]					
	$^3G^o_5$	34349.12[A]	22107.93[A]	22282.900[a]	1.200[A,B,C]	1.200[A]	1.197[a]
		36498.47[B]	21982.01[B]	22269[b]		1.199[B]	
		34188.45[C]					
4f5d	$^3D^o_1$	35406.25[A]	21395.42[A]	21441.730[a]	0.503[A]	0.508[A]	0.542[a]
		37453.79[B]	22982.69[B]	21477[b]	0.501[B]	0.591[B]	
		35168.59[C]			0.512[C]		
	$^3D^o_2$	35923.09[A]	22032.81[A]	22106.020[a]	1.170[A]	1.159[A]	1.167[a]
		37936.33[B]	23003.68[B]	22112[b]	1.169[B,C]	1.195[B]	
		35808.76[C]					
	$^3D^o_3$	36203.19[A]	22475.18[A]	22537.300[a]	1.264[A]	1.305[A]	1.288[a]
		38173.89[B]	23296.42[B]	22483[b]	1.270[B]	1.251[B]	
		36085.58[C]			1.266[C]		
4f5d	$^3P^o_0$	39198.12[A]	22445.78[A]	22683.700[a]			
		40330.43[B]	22463.20[B]	22674[b]			
		38565.29[C]					
	$^3P^o_1$	39440.20[A]	22667.40[A]	22705.150[a]	1.500[A]	1.481[A]	1.431[a]
		40455.15[B]	22524.24[B]	22690[b]	1.498[B]	1.345[B]	
		38560.21[C]			1.485[C]		
	$^3P^o_2$	40081.21[A]	23571.92[A]	23246.930[a]	1.497[A]	1.489[A]	1.459[a]
		40802.14[B]	21850.66[B]	23294[b]	1.492[B,C]	1.337[B]	
		39052.77[C]					
4f5d	$^1F^o_3$	38465.61[A]	24240.21[A]	24552.700[a]	1.061[A]	1.024[A]	1.034[a]
		40442.67[B]	22482.21[B]	24569[b]	1.057[B]	1.055[B]	
		38356.86[C]			1.059[C]		

Table 2: Continued.

Levels		E (cm^{-1})			g-Factors		
		This work			This work		
Conf.	Term	MCHF+BP	HFR	Other works	MCHF+BP	HFR	Other works
4f5d	$^1H^o_5$	46448.76[C]	28811.47[A]	28525.710[a]	1.000[C]	1.001[A,B]	1.004[a]
			27193.29[B]	28529[b]			
4f5d	$^1P^o_1$	47396.25[C]	30265.31[A]	30353.330[a]	1.004[C]	1.040[A]	1.074[a]
			21477.10[B]			1.060[B]	
5d6p	$^1D^o_2$	22996.58[A]	24514.82[A]	24462.66[a]	0.969[A]	1.014[A]	0.887[a]
		19478.98[B]	24310.90[B]	24567[b]	1.011[B]	1.017[B]	
		22618.34[C]			0.975[C]		
5d6p	$^3D^o_1$	24485.41[A]	25907.37[A]	25973.37[a]	0.502[A]	0.579[A]	0.782[a]
		20646.65[B]	25815.48[B]	25839[b]	0.500[B]	0.507[B]	
		23978.78[C]			0.512[C]		
	$^3D^o_2$	25339.58[A]	26457.83[A]	27388.11[a]	1.161[A,B]	1.133[A]	1.168[a]
		21467.30[B]	26411.29[B]	27362[b]	1.139[C]	1.120[B]	
		24934.60[C]					
	$^3D^o_3$	26382.52[A]	26950.18[A]	28315.25[a]	1.323[A]	1.316[A]	1.308[a]
		22400.30[B]	26951.83[B]	28290[b]	1.332[B]	1.312[B]	
		25902.53[C]			1.316[C]		
5d6p	$^1P^o_1$	—	26059.89[A]	—	—	0.955[A]	—
			30735.20[B]			1.064[B]	
5d6p	$^3F^o_2$	27730.01[A]	27524.69[A]	26414.01[a]	0.702[A]	0.691[A]	0.825[a]
		23795.02[B]	27633.61[B]	26409[b]	0.700[B]	0.705[B]	
		27441.41[C]			0.693[C]		
	$^3F^o_3$	28937.43[A]	27941.30[A]	26837.66[a]	1.083[A,B,C]	1.098[A]	1.088[a]
		24648.21[B]	28199.61[B]	26828[b]		1.103[B]	
		28616.27[C]					
	$^3F^o_4$	30401.18[A]	28617.50[A]	28565.40[a]	1.248[A,C]	1.251[A,B]	1.245[a]
		26075.37[B]	29206.78[B]	28531[b]	1.138[B]		
		30028.17[C]					
5d6p	$^3P^o_0$	27489.54[A]	31804.81[A]	31785.82[a]			
		23324.32[B]	32009.00[B]	31797[b]			
		27777.75[C]					
	$^3P^o_1$	27767.31[A]	32243.52[A]	32160.99[a]	1.498[A]	1.497[A]	1.492[a]
		23622.98[B]	32711.11[B]	32134[b]	1.500[B]	1.437[B]	
		27808.39[C]			1.473[C]		
	$^3P^o_2$	28480.17[A]	33269.26[A]	29593[b]	1.469[A]	1.501[A]	—
		24351.70[B]	33441.59[B]		1.460[B]	1.500[B]	
		28624.94[C]			1.482[C]		
5d6p	$^1F^o_3$	34048.66[A]	32144.41[A]	32201.05[a]	0.999[A]	1.002[A]	1.005[a]
		31107.39[B]	32749.00[B]	32273[b]	1.000[B]	1.003[B]	
		33748.76[C]			0.997[C]		
6s6p	$^3P^o_0$	36704.74[A]	27560.27[A]	27545.850[a]			
		32174.15[B]	28370.01[B]	27563[b]			
	$^3P^o_1$	37150.85[A]	28103.04[A]	28154.550[a]?	1.498[A]	1.438[A]	1.267[a]
		32612.03[B]	28403.35[B]	28147[b]	1.501[B]	1.496[B]	
	$^3P^o_2$	37997.38[A]	29477.41[A]	29498.050[a]?	1.494[A]	1.500[A]	1.471[a]
		33501.99[B]	28508.94[B]	33133[b]	1.491[B]	1.501[B]	
6s6p	$^1P^o_1$	—	45700.40[A]	45692.170[a]	—	1.002[A]	0.999[a]

Table 2: Continued.

Levels		E (cm^{-1})			g-Factors		
		This work		Other works	This work		Other works
Conf.	Term	MCHF+BP	HFR		MCHF+BP	HFR	
			45953.40[B]	45702[b]		1.121[B]	
4f7s	$^3F^o_2$	—	60463.77[B]	—	—	0.667[B]	—
	$^3F^o_3$	—	60470.13[B]	—	—	1.048[B]	—
	$^3F^o_4$	—	61873.10[B]	—	—	1.250[B]	—
4f7s	$^1F^o_3$	—	61880.70[B]	—	—	1.036[B]	—
4f6d	$^3F^o_2$	—	57457.37[B]	—	—	0.798[B]	—
	$^3F^o_3$	—	59105.69[B]	—	—	1.121[B]	—
	$^3F^o_4$	—	61261.54[B]	—	—	1.135[B]	—
4f6d	$^1G^o_4$	—	59353.91[B]	—	—	1.037[B]	—
4f6d	$^3G^o_3$	—	57698.08[B]	—	—	0.854[B]	—
	$^3G^o_4$	—	60092.42[B]	—	—	0.998[B]	—
	$^3G^o_5$	—	61115.66[B]	—	—	1.082[B]	—
4f6d	$^3D^o_1$	—	58144.14[B]	—	—	0.823[B]	—
	$^3D^o_2$	—	59943.80[B]	—	—	1.028[B]	—
	$^3D^o_3$	—	61591.58[B]	—	—	1.177[B]	—
4f6d	$^3H^o_4$	—	58359.62[B]	—	—	0.930[B]	—
	$^3H^o_5$	—	60449.51[B]	—	—	1.081[B]	—
	$^3H^o_6$	—	62719.38[B]	—	—	1.167[B]	—
4f6d	$^3P^o_0$	—	60580.29[B]	—	—		
	$^3P^o_1$	—	60380.02[B]	—	—	1.088[B]	—
	$^3P^o_2$	—	59703.78[B]	—	—	1.279[B]	—
4f6d	$^1F^o_3$	—	59802.99[B]	—	—	1.015[B]	—
4f6d	$^1D^o_2$	—	61840.89[B]	—	—	1.233[B]	—
4f6d	$^1P^o_1$	—	62234.11[B]	—	—	1.106[B]	—
4f6d	$^1H^o_5$	—	62355.62[B]	—	—	1.071[B]	—
5d7p	$^3D^o_1$	—	44866.71[B]	—	—	0.749[B]	—
	$^3D^o_2$	—	44866.75[B]	—	—	1.141[B]	—
	$^3D^o_3$	—	47740.96[B]	—	—	1.267[B]	—
5d7p	$^3F^o_2$	—	44842.48[B]	—	—	0.691[B]	—
	$^3F^o_3$	—	44879.84[B]	—	—	1.068[B]	—
	$^3F^o_4$	—	47724.49[B]	—	—	1.251[B]	—
5d7p	$^3P^o_0$	—	44877.71[B]	—	—		
	$^3P^o_1$	—	44424.70[B]	—	—	1.073[B]	—
	$^3P^o_2$	—	47745.11[B]	—	—	1.271[B]	—
5d7p	$^1D^o_2$	—	47754.57[B]	—	—	1.230[B]	—
5d7p	$^1F^o_3$	—	47767.78[B]	—	—	1.083[B]	—
5d7p	$^1P^o_1$	—	48313.70[B]	—	—	1.057[B]	—
6s7p	$^3P^o_0$	—	59907.82[B]	—	—		
	$^3P^o_1$	—	60242.28[B]	—	—	1.451[B]	—
	$^3P^o_2$	—	61529.70[B]	—	—	1.495[B]	—
6s7p	$^1P^o_1$	—	63316.70[B]	—	—	1.033[B]	—

[a]Reference [28], [b]reference [12], ? reference [28].

good for 5d6s ^{3}D levels obtained from calculation C and 5d6s ^{1}D level obtained from calculation A. The result obtained from calculation D for 6s^2 level and the results obtained from calculation A for 6p^2 are in agreement when comparing with others. The results obtained from calculations A and B are also somewhat in agreement for 5d6d and 6s6d levels. 4s6s, 5d6p, and 5d6p levels are good in agreement with others. The 4f5d level is somewhat poor according to other works. It can be said that these cases occur due to unfilled d and, in particular, f subshells. The configuration including these

subshells complicates the calculations in the MCHF method. Results that obtained the Landé g-factors are in quite good agreement with others.

We have studied with two configuration sets (in Table 1) for considering correlation effects in the HFR calculations performed using Cowan's computer code [45]. These configuration sets are also given in Table 1. This approach, although based on the Schrödinger equation, includes the relativistic effects like the mass-velocity corrections and the Darwin contribution beside the spin-orbit effect. In these calculations, the HFR method was combined with a least-squares optimization routine minimizing the discrepancies between observed and calculated energy levels. The scaling factors of the Slater parameters (F^k and G^k) and of configuration interaction integrals (R^k) were chosen equal to 0.75 for calculation A and 0.70 for calculation B, while the spin-orbit parameters were left at their ab initio values. These low values of the scaling factors have been suggested by Cowan for neutral heavy elements [30]. In Table 1, it is taken into account the configuration sets including core [Xe] for calculations A and B of La II. The energies and the Landé g-factors for $5d^2$, 5d6s, $6s^2$, 4f6p, 5d7s, 5d6d, $4f^2$, $6p^2$, 6s6d, 6s7s, 4f6s, 4f5d, 5d6p, 6s6p, 4f7s, 4f6d, 5d7p, and 6s7p excited levels are presented in Table 2. The agreement between our energies and the Landé g-factors from the HFR calculation obtained according to A and B configuration sets and other works is very good.

These energy data and the Landé g-factors for La II can be useful in investigations of some radiative properties and interpretation of many levels of La II. Because magnetic fields play a major role in many scientific areas such as astrophysics, the calculation of the Landé g-factor is important. The experimental values for Landé g-factors of rare-earth elements are far from being complete. We hope that the results reported in this work will be useful in the interpretation of atomic spectra of La II. Many feature characteristics of the spectra of neutral atom or ions of lanthanides remain preserved for lanthanide ions implemented in crystals. This is one reason for the wide interest in the application of lanthanides as active media in lasers. In addition, knowledge of electronic levels of lanthanides is important in astrophysics, since it allows precise determination of the abundance of particular elements. Also, the analysis of electronic levels is very important for a description of the interaction in creating chemical bonds or crystalline lattice. Consequently, we hope that our results obtained using the HFR and MCHF methods will be useful for other works in the future for La II spectra.

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