The Hyperfine Structure Calculations of Some Excited Levels for ^{139}La I

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We calculated hyperfine structure constants of the $5d6s^2$, $5d^26s$, $5d^3$, $5d^27s$, $5d6s7s$, $5d6p^2$, $4f^25d$, $4f6s6p$, $5d6s6p$, $5d^26p$, $4f5d6s$ and $4f5d^2$ levels for ^{139}La I ($Z = 57$). The calculations are based upon the multiconfiguration Hartree–Fock method within the framework of the Breit–Pauli relativistic corrections. Moreover, the results obtained were compared with other available calculations and experiments.

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1. Introduction

The neutral lanthanum atom, which is the first member of the rare-earth elements, comes just before the $4f$ subshell and has the low-lying levels $(5d + 6s)^3$. They interact with each other because of a number of closely spaced levels. Lanthanum has two naturally occurring isotopes ^{138}La (0.085%) and ^{139}La (99.910%). ^{139}La has nuclear spin of 7/2, magnetic dipole moment of $\mu_I = 2.783\,045\,5(9)\mu_N$ and a electric quadrupole moment of $Q = 0.20(1)$ b [1].

The hyperfine structure of La I has been investigated in the past by different experimental techniques and theoretical methods (atomic-beam magnetic resonance method, the laser-rf double-resonance and laser induced-fluorescence spectroscopy with atomic-beam, Doppler-free intermodulated fluorescence, Doppler-limited laser-induced fluorescence and optogalvanic spectroscopy, diode-laser-initiated resonance-ionization and mass-spectrometric detection, optical interference spectroscopy, the method of laser induced fluorescence in a hollow cathode discharge, and multiconfiguration Dirac–Fock (MCDF) *ab initio* calculations) [2–17].

Although much research has been done on the hyperfine structure of neutral lanthanum, many configurations (especially, highly excited levels) are yet to be investigated, and theoretical information about this atom is still far from complete because of the complex nature of atomic spectra. We have presented here some results which belong to hyperfine structure of our continuing program for the isotope ^{139}La using MCHF code of Fischer [18]. The ground-state level of neutral lanthanum is $5d6s^2\ ^2D_{3/2}$. In order to consider correlation effects, we have selected the $5d6snp$, $5d^2np$, np^3, ns^27p, $4f5dns$ ($n = 6, 7$), $4fnd^2$ ($n = 5, 6$), $6s^26p$, $6p7s^2$, $5d6p7s$, $5d7s7p$, $6s6p7s$, $6s7s7p$, $6p^27p$, and $6p7p^2$ configurations for odd-parity levels and the $5dns^2$, $5d^2ns$, $5dnp^2$, $6snp^2$, $4f6snp$ ($n = 6, 7$), $4f^25d$, $4f6p7s$, $4f7s7p$, $5d^3$, $6p^27s$, $6s7s^2$, $6s^27s$, $7s7p^2$, $5d6s7s$, $5d6p7p$, $6s6p7p$, and $6p7s7p$ configurations for even-parity levels outside the core [Xe] in neutral lanthanum. We have performed large-scale multiconfiguration Hartree–Fock (MCHF) and configuration interaction (CI) calculations for $5d6s^2$, $5d^26s$, $5d^3$, $5d^27s$, $5d6s7s$, $5d6p^2$, $4f^25d$, $4f6s6p$, $5d6s6p$, $5d^26p$, $4f5d6s$ and $4f5d^2$ levels. Our earlier works for this atom consist of electric dipole transitions and lifetimes for some excited levels [19, 20].

The purpose of the present work is to extend the hyperfine structure constants of magnetic dipole interaction — A and electric quadrupole interaction — B, using possible large configuration set. Thus it will provide to information on the hyperfine structure and help to deadly analyze the La I spectrum.

2. Method of calculation

In this work, the wave functions are obtained using MCHF method [21]. In this method, the wave function Ψ for a state labelled γLS is expanded in terms of configuration state functions (CSFs) with the same LS term

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

γ and c_i represent here the configuration with any other quantum numbers and mixing coefficients, respectively. In a configuration interaction calculation, the wave function is expanded in CSFs, but only the mixing (or expansion) coefficients are to be determined.

To consider the relativistic effects, the Breit–Pauli Hamiltonian can be written

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

where $H_{\rm NR}$ is nonrelativistic many-electron Hamiltonian and $H_{\rm RS}$ is relativistic shift operator including mass

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correction, the one- and two-body Darwin terms, j--independent orbit–orbit and spin–spin contact terms. Fine structure operator ($H_{\rm FS}$) includes the spin–orbit, spin–other–orbit and spin–spin interaction terms. Thus the total wave function can be written in the form

$$\Psi(\gamma JM_J) = \sum_{i=1}^{M} c_i \Phi(\gamma_i L_i S_i JM_J). \tag{3}$$

$\Phi(\gamma LSJM_J)$ are here LSJ coupled CSFs. In the calculations, the CSFs are taken from nonrelativistic MCHF run, and only mixing coefficients are optimized. The matrix eigenvalue problem becomes

$$\boldsymbol{Hc} = E\boldsymbol{c}, \tag{4}$$

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

$$H_{ij} = \langle \gamma_i L_i S_i JM_J | H_{\rm BP} | \gamma_j L_j S_j JM_J \rangle \tag{5}$$

and $\boldsymbol{c}$ the column vector of the expansion coefficients. The Breit–Pauli Hamiltonian is a first-order perturbation correction to the nonrelativistic Hamiltonian.

The fine-structure levels of atoms in many cases are not single levels. They consist of closely spaced levels, the so-called hyperfine structure. The hyperfine structure of the atomic energy levels is caused by interaction between the electrons and the electromagnetic multipole moments of the nucleus. The contribution to the Hamiltonian can be represented by an expansion in multipoles of order K,

$$H_{\rm hfs} = \sum_{K\geq 1} \boldsymbol{T}^{(K)} \cdot \boldsymbol{M}^{(K)}. \tag{6}$$

$\boldsymbol{T}^{(K)}$ and $\boldsymbol{M}^{(K)}$ are here spherical tensor operators of rank K in the electronic and nuclear space, respectively. The $K = 1$ term represents the magnetic dipole interaction and $K = 2$ term represents the electronic quadrupole interaction. The hyperfine interaction couples the electronic ($\boldsymbol{J}$) and nuclear ($\boldsymbol{I}$) angular momentum to a total angular momentum $\boldsymbol{F} = \boldsymbol{I} + \boldsymbol{J}$, and leads to a splitting of the fine structure levels. The splitting is often given in terms of the magnetic dipole and electric quadrupole interaction constants (A_J and B_J),

$$A_J = \frac{\mu_I}{I} \frac{1}{[J(J+1)(2J+1)]^{1/2}} \times \left\langle \gamma_J J \left\| T^{(1)} \right\| \gamma_J J \right\rangle, \tag{7}$$

$$B_J = 2Q \left[\frac{J(2J-1)}{(J+1)(2J+1)(2J+3)} \right]^{1/2} \times \left\langle \gamma_J J \left\| T^{(2)} \right\| \gamma_J J \right\rangle, \tag{8}$$

where $\boldsymbol{I}$ is the nuclear spin, μ_I is the nuclear magnetic dipole moment, and Q is the nuclear quadrupole moment, and $\boldsymbol{T}^{(1)}$ and $\boldsymbol{T}^{(2)}$ represent electronic tensor operators (see, e.g., [21]). The magnetic dipole operator ($\boldsymbol{T}^{(1)}$) represents the magnetic field due to the electrons at the site of the nucleus. This operator includes the field caused by orbital motion of the electrons, called the orbital term, dipole field due to the spin motions of the electron, called the spin–dipole term and the contact interaction between the nucleus and the electron spin occurring only for s electrons. The electric quadrupole operator ($\boldsymbol{T}^{(2)}$) represents the electric-field gradient at the site of nucleus.

TABLE I

Hyperfine structure (HFS) constants, A and B, for ^{139}La I (for even-parity levels). Footnotes after Table II.

Levels			HFS constants [MHz]					
			A			B		
configuration	term	J	this work	other works		this work	other works	
				exp.	MCDF		exp.	MCDF
$5d6s^2$	^2D	3/2	143.27	141.1959[a] 147(6)[e]	111.23[a]	27.57	44.781[a]	29.59[a]
		5/2	184.10	182.1706[a] 210(5)[e] 183(5)[g]	235.64[a]	37.57	54.213[a]	32.21[a]
$5d^2(^3F)6s$	^4F	3/2	−322.87	−480.292[a] −480.312[b] −480.66(28)[c] −480(6)[e] −479(6)[g] −480.224(8)[h]	−398.55[a]	11.66	15.188[a] 15.082[b] 16.7(2.1)[c] 14.2 ± 0.2[h]	14.84[a]
		5/2	246.44	300.563[a] 300.56[b] 300.58(18)[c] 300(5)[e,g] 300.631(8)[h]	250.19[a]	11.62	10.873[a] 10.87[b] 11.3(2.8)[c] 14.0 ± 0.3[h]	11.41[a]

TABLE I (cont.)

Levels			HFS constants [MHz]					
			A			B		
configuration	term	J	this work	other works		this work	other works	
				exp.	MCDF		exp.	MCDF
		7/2	379.86	462.868[a] 462.87[b] 463.25(32)[c] 459(8)[e] 459(4)[g] 462.889(7)[h]	392.78[a]	16.08	17.925[a] 17.93[b] 23.3(5.9)[c] 19.3 ± 0.2[h]	15.45[a]
		9/2	410.92	489.534[a] 489.534[b] 489.71(22)[c] 495(4)[e] 489.533(2)[h]	451.32[a]	24.22	32.180[a] 32.180[b] 32.6(6.1)[c] 31.9 ± 0.2[h]	26.17[a]
$5d^2(^3P)6s$	^4P	1/2	2137.07	2460.161[a] 2460.173(70)[h]	1913.46[a]	0.00	0[a]	0[a]
		3/2	822.32	929.618[a] 936(6)[e] 929.6 ± 0.2[h]	844.26[a]	23.27	37.221[a] 37.2 ± 2.5[h]	28.58[a]
		5/2	604.59	802.172[a] 810(5)[e,g] 801.9 ± 0.5[h]	731.87[a]	−17.17	−34.186[a] −40 ± 8[h]	−36.09[a]
$5d^2(^3F)6s$	^2F	5/2	209.15	304.372[a] 303(5)[g] 304.381(4)[h]	271.92[a]	21.26	28.091[a] 27.8 ± 0.1[h]	20.04[a]
		7/2	−11.01	−197.064[a] −197(4)[e,g] −197.068(7)[h]	−12.80[a]	27.46	40.754[a] 41.4 ± 0.2[h]	29.02[a]
$5d^2(^1G)6s$	^2G	7/2	−98.07	−292.267[a] −300(4)[e]	−178.47[a]	79.38	67.537[a]	76.66[a]
		9/2	333.93	559.812[a]	431.58[a]	70.67	202.638[a]	85.78[a]
$5d^2(^1S)6s$	^2S	1/2	2543.29	–	–	0.00	–	–
$5d^3$	^4F	3/2	109.78	445.086[a]	176.15[a]	−12.02	−16.068[a]	−12.02[a]
		5/2	182.90	97.510[a]	105.89[a]	−14.69	−16.521[a]	−12.91[a]
		7/2	102.15	−19.103[a]	86.06[a]	−14.33	−20.898[a]	−17.80[a]
		9/2	155.31	−63.829[a]	82.06[a]	−3.29	−27.385[a]	−23.87[a]
$5d^3$	^4P	1/2	−110.46	–	–	0.00	–	–
		3/2	74.03	–	–	-26.67	–	–
		5/2	42.97	–	–	32.72	–	–
$5d^3$	$^2D1$	3/2	197.08	–	–	46.42	–	–
		5/2	107.85	–	–	55.60	–	–
$5d^3$	^2P	1/2	128.12	–	–	0.00	–	–
		3/2	61.99	–	–	-19.64	–	–
$5d^3$	^2D	3/2	156.69	–	–	-29.35	–	–
		5/2	135.79	–	–	-33.61	–	–
$5d^3$	^2G	7/2	133.92	–	–	36.80	–	–
		9/2	154.02	–	–	43.79	–	–
$5d^3$	^2F	5/2	129.85	–	–	31.65	–	–
		7/2	132.71	–	–	21.68	–	–

TABLE I (cont.)

Levels			HFS constants [MHz]					
			A			*B*		
configuration	term	*J*	this work	other works		this work	other works	
				exp.	MCDF		exp.	MCDF
$5d^3$	^2H	9/2	135.09	–	–	61.48	–	–
		11/2	129.71	–	–	73.14	–	–
$5d^2(^1S)7s$	^2S	1/2	4669.09	–	–	0.00	–	–
$5d^2(^1G)7s$	^2G	7/2	−376.87	–	–	86.78	–	–
		9/2	692.27	–	–	101.61	–	–
$5d^2(^3P)7s$	^4P	1/2	2796.84	–	–	0.00	–	–
		3/2	1196.92	–	–	28.80	–	–
		5/2	997.92	–	–	-30.94	–	–
$5d6s(^3D)7s$	^2D	3/2	62.73	–	–	28.60	–	–
		5/2	273.91	–	–	35.67	–	–
$5d6s(^3D)7s$	^4D	1/2	−1963.47	–	–	0.00	–	–
		3/2	872.90	–	–	2.32	–	–
		5/2	1166.93	–	–	24.76	–	–
		7/2	1027.58	–	–	51.61	–	–
$5d6p^2(^1S)$	^2D	3/2	295.82	–	–	218.20	–	–
		5/2	254.54	–	–	263.52	–	–
$5d6p^2(^1D)$	^2S	1/2	2233.73	–	–	0.00	–	–
$5d6p^2(^1D)$	^2P	1/2	−883.20	–	–	0.00	–	–
		3/2	437.84	–	–	−89.87	–	–
$5d6p^2(^1D)$	^2D	3/2	436.12	–	–	−86.54	–	–
		5/2	968.05	–	–	−42.47	–	–
$4f^2(^1S)5d$	^2D	3/2	377.21	–	–	94.64	–	–
		5/2	291.60	–	–	154.41	–	–
$4f^2(^1D)5d$	^2D	3/2	85.88	–	–	−18.45	–	–
		5/2	88.71	–	–	27.32	–	–
$4f^2(^1G)5d$	^2D	3/2	48.56	–	–	8.74	–	–
		5/2	130.01	–	–	32.96	–	–
$4f^2(^1G)5d$	^2F	5/2	73.68	–	–	−8.72	–	–
		7/2	71.55	–	–	−12.20	–	–
$4f^2(^3P)5d$	^4D	1/2	48.45	–	–	0.00	–	–
		3/2	88.31	–	–	−25.57	–	–
		5/2	109.36	–	–	−19.64	–	–
		7/2	89.67	–	–	58.05	–	–
$4f^2(^3F)5d$	^2F	5/2	86.75	–	–	−17.85	–	–
		7/2	78.47	–	–	−12.59	–	–
$4f^2(^3F)5d$	^4P	1/2	93.90	–	–	0.00	–	–
		3/2	314.79	–	–	58.92	–	–
		5/2	46.53	–	–	−4.11	–	–
$4f^2(^3F)5d$	^4F	3/2	130.36	–	–	0.79	–	–
		5/2	99.84	–	–	3.72	–	–
		7/2	73.65	–	–	1.52	–	–
		9/2	64.97	–	–	4.87	–	–

TABLE I (cont.)

Levels			HFS constants [MHz]					
			A			B		
configuration	term	J	this work	other works		this work	other works	
				exp.	MCDF		exp.	MCDF
$4f6s(^1F)6p$	^2D	3/2	−53.14	–	–	107.19	–	–
		5/2	306.69	–	–	247.99	–	–
$4f6s(^1F)6p$	^2G	7/2	379.21	–	–	177.46	–	–
		9/2	626.41	–	–	405.35	–	–
$4f6s(^3F)6p$	^2F	5/2	−8.09	–	–	−81.65	–	–
		7/2	565.05	–	–	−70.17	–	–
$4f6s(^3F)6p$	^2G	7/2	205.57	–	–	311.80	–	–
		9/2	218.44	–	–	376.03	–	–
$4f6s(^3F)6p$	^4D	1/2	−1774.61	–	–	0.00	–	–
		3/2	126.45	–	–	−79.09	–	–
		5/2	457.31	–	–	−62.90	–	–
		7/2	434.61	–	–	29.34	–	–

TABLE II

Hyperfine structure (HFS) constants, A and B, for ^{139}La I (for odd-parity levels).

Levels			HFS constants [MHz]					
			A			B		
configuration	term	J	this work	other works		this work	other works	
				exp.	MCDF		exp.	MCDF
$5d6s(^3D)6p$	$^4F^o$	3/2	−81.93	−351.3(3)[b] −348.8(1.8)[d] −471(6)[g]	–	13.09	75(5)[b]	–
		5/2	239.54	333(1)[b] 334.4(2.0)[d]	–	35.62	20(5)[b]	–
		7/2	438.90	673.6(3)[b] 673.2(1.1)[d]	–	49.23	60(10)[b]	–
		9/2	416.81	613.3(4)[b] 611.0(3.1)[d]	–	93.92	150(15)[b]	–
$5d6s(^3D)6p$	$^4D^o$	1/2	−600.20	−581.4(1.3)[b] −579.0(0.9)[d]	–	0.00	0[b]	–
		3/2	261.01	586.1(3)[b] 589.3(3.3)[d]	–	26.56	53(5)[b]	–
		5/2	365.92	589.5(2.2)[d]	–	1.42	–	–
		7/2	490.06	585.9(3.5)[d]	–	−7.98	–	–
$5d6s(^3D)6p$	$^4P^o$	1/2	1926.43	2887.7(2.6)[d]	–	0.00	–	–
		3/2	770.34	1328.6(2.9)[d]	–	3.24	–	–
		5/2	579.97	633.3(1.2)[d] 661.4(6)[f]	–	19.27	18(10)[d]	–
$5d6s(^3D)6p$	$^2P^o$	1/2	358.40	–	–	0.00	–	–
		3/2	188.61	–	–	14.80	–	–
$5d6s(^3D)6p$	$^2D^o$	3/2	260.27	–	–	3.66	–	–
		5/2	48.37	–	–	14.24	–	–

TABLE II (cont.)

Levels			HFS constants [MHz]					
			A			B		
configuration	term	J	this work	other works		this work	other works	
				exp.	MCDF		exp.	MCDF
$5d6s(^1D)6p$	$^2P^o$	1/2	−172.71	126.88(56)[c] 132.6(2.0)[d] 145(7)[g]	–	0.00	0.0[d]	–
		3/2	420.80	−41.81(15)[c] −38.7(5.2)[d] −48(6)[g]	–	19.92	1.8(1.2)[c]	–
$5d^2(^1G)6p$	$^2F^o$	5/2	154.71	–	–	63.56	–	–
		7/2	106.77	–	–	68.80	–	–
$5d^2(^3P)6p$	$^2D^o$	3/2	133.93	478.5(1.9)[d]	–	2.08	18(16)[d]	–
		5/2	118.78	100(5)[e]	–	14.12	–	–
$5d^2(^3F)6p$	$^2F^o$	5/2	6.80	–	–	29.75	–	–
		7/2	83.78	–	–	23.20	–	–
$5d^2(^3F)6p$	$^4D^o$	1/2	244.87	524.8(9.0)[d]	–	0.00	0.0[d]	–
		3/2	155.32	149.5(3.2)[d]	–	2.34	−45(35)[d]	–
		5/2	216.31	45.4(6.5)[d]	–	7.01	0(20)[d]	–
		7/2	188.99	−28.1(0.5)[d]	–	18.76	49(20)[d]	–
$5d^2(^3F)6p$	$^4G^o$	5/2	342.30	539.9(3.3)[d] 540(5)[g]	–	28.76	–	–
		7/2	169.93	223(4)[g]	–	39.44	–	–
		9/2	136.17	110.1(1.0)[d]	–	49.07	85(30)[d]	–
		11/2	111.08	–	–	61.13	–	–
$5d^2(^1S)6p$	$^2P^o$	1/2	307.91	–	–	0.00	–	–
		3/2	61.61	–	–	32.05	–	–
$5d^2(^1D)6p$	$^2D^o$	3/2	71.24	132.9(1.6)[d]	–	−21.93	–	–
		5/2	160.34	344.3(5.0)[d]	–	−24.36	−71(40)[d]	–
$5d^2(^1G)6p$	$^2G^o$	7/2	139.77	75.8[a] 88(4)[e]	–	46.01	45.0[a]	–
		9/2	168.68	186.7(2.0)[d]	–	58.84	35(30)[d]	–
$5d^2(^1G)6p$	$^2H^o$	9/2	155.00	–	–	123.50	–	–
		11/2	138.48	–	–	138.40	–	–
$5d^2(^3P)6p$	$^2S^o$	1/2	5.42	–	–	0.00	–	–
$5d^2(^3P)6p$	$^4S^o$	3/2	1.71	−199.77(8)[c] −199.6(1.0)[d] −232(6)[e] −235(6)[g]	–	0.095	2.75(64)[c] 14(10)[d]	–
$5d^2(^3P)6p$	$^4D^o$	1/2	220.27	290.3(2.0)[d]	–	0.00	0.00[d]	–
		3/2	125.90	105.1(2.0)[d] 156(6)[e]	–	−0.23	−21(15)[d]	–
		5/2	112.51	324.8(1.7)[d]	–	−7.13	−44(15)[d]	–
		7/2	149.03	70(2)[b] 68.1(2.0)[d] 77(4)[e]	–	8.49	13(20)[b] 70(20)[d]	–
$5d^2(^3P)6p$	$^2P^o$	1/2	232.42	274.8(3.4)[d]	–	0.00	0.00[d]	–
		3/2	59.26	–	–	4.61	–	–
$5d^2(^3F)6p$	$^2D^o$	3/2	59.14	142.1(0.6)[d]	–	8.93	–	–
		5/2	144.41	−58.1(0.6)[d] −58.7(3)[f]	–	15.88	–	–

TABLE II (cont.)

Levels			HFS constants [MHz]					
			A			B		
configuration	term	J	this work	other works		this work	other works	
				exp.	MCDF		exp.	MCDF
$5d^2(^3F)6p$	$^2G^o$	7/2	156.40	283.9(3)[b] 284.7(1.0)[d]	–	32.61	60(25)[b] 44(27)[d]	–
		9/2	119.34	–	–	40.83	–	–
$5d^2(^3F)6p$	$^4F^o$	3/2	160.14	88.67(10)[c] 83.6(10)[d] 91(6)[e]	–	−2.06	−4.0(1.8)[c]	–
		5/2	287.18	258.76(26)[c] 265(5)[g]	–	−2.10	6.9(4.1)[c]	–
		7/2	204.08	195.59(8)[c] 194.5(1.6)[d] 193(8)[e]	–	8.15	1.8(3.1)[c]	–
		9/2	176.09	92.38(4)[c] 94.9(1.0)[d] 96(4)[e]	–	10.49	−10.1(3.2)[c] −20(15)[d]	–
$5d^2(^3P)6p$	$^4P^o$	1/2	−1.48	−296.8[a] −297.3(1.5)[d]	–	0.00	0[a] 0.00[d]	–
		3/2	51.01	–	–	−4.87	–	–
		5/2	94.860	100.7[a] 103.2(2.2)[d]	–	13.81	−5.6[a] −29(20)[d]	–
$4f5d(^1D)6s$	$^2D^o$	3/2	−84.09	–	–	−2.01	–	–
		5/2	197.02	–	–	14.72	–	–
$4f5d(^1F)6s$	$^2F^o$	5/2	232.65	–	–	43.06	–	–
		7/2	248.33	–	–	53.67	–	–
$4f5d(^1G)6s$	$^2G^o$	7/2	−21.67	188.4(1.7)[d] 182.8(2)[f]	–	26.47	17(15)[d]	–
		9/2	335.98	373.1(0.5)[d]	–	10.95	18(10)[d]	–
$4f5d(^1H)6s$	$^2H^o$	9/2	65.01	−97.5(7.0)[d]	–	77.01	–	–
		11/2	209.87	423.5(4.5)[d]	–	91.77	–	–
$4f5d(^3D)6s$	$^2D^o$	3/2	172.71	–	–	22.62	–	–
		5/2	112.50	–	–	0.93	–	–
$4f5d(^3F)6s$	$^4F^o$	3/2	−244.04	−228.9(2.2)[d]	–	−11.07	30(11)[d]	–
		5/2	233.64	–	–	−15.10	–	–
		7/2	245.25	391.0(0.5)[d]	–	−9.74	−42(19)[d]	–
		9/2	300.18	414.3(2.0)[d]	–	6.13	40(20)[d]	–
$4f5d(^3G)6s$	$^2G^o$	7/2	163.64	–	–	44.24	–	–
		9/2	96.76	–	–	54.46	–	–
$4f5d(^3G)6s$	$^4G^o$	5/2	-23.18	−147.7(1.6)[d]	–	34.72	17(20)[d]	–
		7/2	127.33	358.0(1.6)[d]	–	33.74	50(13)[d]	–
		9/2	171.41	393.0(5.2)[d]	–	34.04	120(60)[d]	–
		11/2	159.26	–	–	39.54	–	–
$4f5d(^3H)6s$	$^2H^o$	9/2	163.09	–	–	64.81	–	–
		11/2	1.05	17.3(0.4)[d]	–	72.20	–	–
$4f5d(^3H)6s$	$^4H^o$	7/2	−107.53	−134.1(4.0)[d]	–	69.78	72(30)[d]	–
		9/2	171.68	–	–	67.93	–	–
		11/2	251.55	–	–	75.31	–	–
		13/2	275.59	–	–	88.13	–	–
$4f5d^2(^1D)$	$^2P^o$	1/2	143.85	–	–	0.00	–	–
		3/2	50.13	–	–	7.08	–	–

TABLE II (cont.)

Levels			HFS constants [MHz]					
			A			*B*		
configuration	term	*J*	this work	other works		this work	other works	
				exp.	MCDF		exp.	MCDF
$4f5d^2(^1D)$	$^2G^o$	7/2	123.72	–	–	24.89	–	–
		9/2	98.24	–	–	43.58	–	–
$4f5d^2(^3P)$	$^4F^o$	3/2	170.33	–	–	39.10	–	–
		5/2	124.62	–	–	40.55	–	–
		7/2	99.20	–	–	53.59	–	–
		9/2	53.35	–	–	77.44	–	–
$4f5d^2(^3P)$	$^4G^o$	5/2	160.40	–	–	23.77	–	–
		7/2	128.51	–	–	23.15	–	–
		9/2	135.99	–	–	29.82	–	–
		11/2	154.60	–	–	45.52	–	–
$4f5d^2(^3F)$	$^4S^o$	3/2	21.98	–	–	−0.17	–	–
$4f5d^2(^3F)$	$^4F^o$	3/2	167.48	–	–	−16.20	–	–
		5/2	114.70	–	–	−11.67	–	–
		7/2	111.04	–	–	−6.82	–	–
		9/2	92.34	–	–	−21.70	–	–
$4f5d^2(^3F)$	$^4G^o$	5/2	146.72	–	–	−5.13	–	–
		7/2	160.36	–	–	0.66	–	–
		9/2	95.64	–	–	−18.99	–	–
		11/2	90.09	–	–	−21.97	–	–

[a]Ref. [7], [b]Ref. [16], [c]Ref. [10], [d]Ref. [17], [e]Ref. [12], [f]Ref. [9], [g]Ref. [13], [h]Ref. [3]

3. Results and discussion

In this work, hyperfine structure constants have been calculated for $5d6s^2$, $5d^26s$, $5d^3$, $5d^27s$, $5d6s7s$, $5d6p^2$, $4f^25d$, $4f6s6p$, $5d6s6p$, $5d^26p$, $4f5d6s$ and $4f5d^2$ excited levels outside core [Xe] in neutral lanthanum (La I) using the MCHF atomic-structure package [18]. The main purpose of this paper was to perform the MCHF + Breit–Pauli calculations for obtaining a hyperfine structure description of ^{139}La spectrum. In Tables I and II the calculated magnetic dipole hyperfine structure constants A and electric quadrupole constants B, and some available hyperfine structure constants from the literature for comparison have been given for these levels. The references for comparison values are typed below the table with superscript lowercase letter. In Tables I and II, results of the hyperfine structure calculations are compared with the experimental and MCDF method [3, 7, 9, 10, 12, 13, 16, 17]. As seen in Tables I and II, some results are in good agreement with others. Agreement for some $5d6s6p$ and $4f5d6s$ levels is somewhat poor. The reason for these poor agreements, probably, is to not consider large configuration set and include core–core and core–valence correlation. It is known that electron correlation and relativistic effects play an important role in the spectra of heavy atoms. However, it is very difficult to consider such effects in the MCHF method because of the complex structure of lanthanum and computer constraints [20].

The spectra of lanthanides analysis provide useful information among other things on the chemical composition of the different types of stars (in particular, in the spectra of peculiar stars) in astrophysics, and accurate atomic data are required in the models used for lamp design and diagnostics [22]. It is known that there are experimentally most levels with unknown energy values in the lanthanum spectra. The presence of hyperfine structure splitting complicates the determination of accurate line position, because these splittings are large enough to produce separate energy levels. In this work new data on hyperfine structure for some levels in ^{139}La I are obtained. These kinds of data are essential inputs to a wide range of problems encountered in many areas of science, such as astrophysics, plasma physics and atmospheric physics, and environmental research. We hope that the results obtained in this work will be useful for the experimental and theoretical works in analyzing lanthanum spectra.

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