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Energies and Lifetimes for Some Excited Levels in La I

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We calculated relativistic energies and Landé factors for $5d6s^2$, $5d^26s$, $5d^3$, $5d6s7s$, $4f6s6p$, $5d6s6p$, $5d^26p$, and $4f5d6s$ levels in neutral lanthanum ($Z = 57$). We also obtained electric dipole transition energies and lifetimes for some excited levels. The calculations are based upon the multiconfiguration Hartree–Fock method within the framework Breit–Pauli relativistic corrections. Moreover, the results obtained were compared with other calculations and experiments.

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1. Introduction

The rare earths consist of two series of elements, lanthanides and actinides, which roughly speaking involve filling of the $4f$ and $5f$ subshells, respectively [1]. The lanthanides are the group of elements with atomic number $Z = 57$ to 71. Atomic calculations belonging to these elements can be said far too much not to exist. The unique properties of lanthanide elements, and also of lanthanum in particular, are a direct result of the small radius of the $4f$ orbital which is smaller than that of the $5s$ electron [2]. The collapse of the $4f$ orbital occurs at lanthanum ($Z = 57$) firstly. Therefore, accurate calculations of wave functions in this atom are extremely complex. In particular, the $4f^N$ configurations make the analysis of the lanthanide spectra extremely complex and time consuming. This collapse has been frequently considered in the literature.

Because of the rich emission spectra of lanthanides in the visible region in outside astrophysics, accurate atomic data are required in the models used for lamp design and diagnostics in the lighting-research community. In addition, the lanthanide ions can be used as a sensitive probe of crystalline structure of the salts [3].

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The latest data belonging to energy levels, oscillator strengths, wavelengths, and transition probabilities for electric multipole transitions of La I can be found in KURUCZ and NIST on web sites [4, 5]. Theoretical knowledge and investigation of some levels concerning the lanthanide atoms have been presented by Cowan [1]. In addition, data related to atomic structure calculations and experiments as energy levels, wavelengths, oscillator strengths, transition probabilities, and lifetimes for electric dipole transitions in lanthanides are reported [6–25].

Recently, Biémont and Quinet performed the radiative lifetime measurements with a time-resolved laser-induced fluorescence technique for some levels of La I, and presented an overview of the recent developments concerning the spectroscopic properties of lanthanide atoms and ions [2, 3].

In this work, energies and Landé factors (g factor) for $5d6s^2$, $5d^26s$, $5d^3$, $5d6s7s$, $4f6s6p$, $5d6s6p$, $5d^26p$, and $4f5d6s$ excited levels outside core [Xe] in neutral lanthanum have been calculated using multiconfiguration Hartree–Fock (MCHF) approximation within the framework Breit–Pauli Hamiltonian for relativistic corrections developed by Fischer et al. [26], and presented in tables for comparison with other works. Transition energies for electric dipole transitions (E1) which combine the states of different parity and lifetimes of some lower lying excited levels among those have been also obtained. Neutral lanthanum (La I) has two stable isotopes, i.e. ^{138}La (0.09%) and ^{139}La (99.91%). 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, $4f5dns$ ($n = 6, 7$), $4fnd^2$ ($n = 5, 6$), $6p7s^2$, $5d6p7s$, $5d7s7p$, $6s6p7s$, $6s7s7p$, $6p^27p$, and $6p7p^2$ configurations for odd-parity levels and the $5dns^2$, $5d^2ns$, $5dnp^2$, $6snp^2$, $4f6snp$ ($n = 6, 7$), $4f^25d$, $4f6p7s$, $4f7s7p$, $5d^3$, $6p^27s$, $6s7s^2$, $7s7p^2$, $5d6s7s$, $5d6p7p$, $6s6p7p$, and $6p7s7p$ configurations for even-parity levels outside the core [Xe] in neutral lanthanum. The aim of this paper performs MCHF calculations for the lower excited states for partially obtaining a description of the La I spectrum.

2. Method of calculation

The MCHF approximation is a configuration interaction (CI) method. In this approximation the MCHF Hamiltonian is used for obtaining the best radial functions for the set of non-relativistic energies of the interacting terms. The wave function is approximated by a linear combination of orthonormal configuration state functions so that

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

In this expansion $\Phi(\gamma_i LS)$, γ_i, and c_i represent configuration state function in LS coupling, configurations, and mixing coefficients of configurations, respectively. Then the non-relativistic energy expression becomes

$$\varepsilon(\gamma LS) = \sum_{i=1}^{M}\sum_{j=1}^{M} c_i c_j \left\langle \Phi(\gamma_i LS)|H|\Phi(\gamma_j LS)\right\rangle$$
$$= \sum_{i=1}^{M}\sum_{j=1}^{M} c_i c_j H_{ij} = \sum_{i=1}^{M} c_i^2 H_{ii} + 2\sum_{i>j}^{M} c_i c_j H_{ij}. \tag{2}$$

The Breit–Pauli Hamiltonian includes relativistic effects. This Hamiltonian can be written as

$$H_{\rm BP} = H_{\rm NR} + H_{\rm RS} + H_{\rm FS}, \tag{3}$$

where $H_{\rm NR}$ is the non-relativistic many-electron Hamiltonian. The relativistic shift operator $H_{\rm RS}$ includes the mass correction, one- and two-body Darwin terms, the spin–spin contact term, and the orbit–orbit term

$$H_{\rm RS} = H_{\rm MC} + H_{\rm D1} + H_{\rm D2} + H_{\rm OO} + H_{\rm SSC}. \tag{4}$$

This operator commutes with $\boldsymbol{L}$ and $\boldsymbol{S}$. The fine-structure operator $H_{\rm FS}$ does not commute with $\boldsymbol{L}$ and $\boldsymbol{S}$ but with total angular momentum $\boldsymbol{J}$, and describes interactions between the spin and orbital angular momenta of the electrons. This operator consists of the spin–orbit interaction, spin–other-orbit interaction, and spin–spin interaction terms

$$H_{\rm FS} = H_{\rm SO} + H_{\rm SOO} + H_{\rm SS}. \tag{5}$$

Then, the Breit–Pauli wave functions are obtained as linear combinations

$$\Psi(\gamma J M_J) = \sum_{i=1}^{M} c_i \, \Phi(\gamma_i L_i S_i J M_J), \tag{6}$$

where $\Phi(\gamma LSJM_J)$ are LSJ coupled configuration state functions (CSFs). In the calculations, the CSFs are taken from non-relativistic MCHF run, and only mixing coefficients are optimized. Then, the matrix eigenvalue problem becomes

$$\boldsymbol{Hc} = E\boldsymbol{c}, \tag{7}$$

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

$$H_{ij} = \langle \gamma_i L_i S_i J M_J | H_{\rm BP} | \gamma_j L_j S_j J M_J \rangle \tag{8}$$

and $c = (c_1, \ldots, c_M)^t$ the column vector of the expansion coefficients. The Breit–Pauli Hamiltonian is a first-order perturbation correction to the non-relativistic Hamiltonian.

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, $\tau_{\gamma' J'}$, of upper level $(\gamma' J')$ is

$$\tau_{\gamma' J'} = \frac{1}{\sum_{\pi k, \gamma J} A^{\pi k}(\gamma' J', \gamma J)}. \tag{9}$$

In the formula (9), $A^{\pi k}$ is the transition probability for emission from the upper level to the lower level in the form

$$A^{\pi k}(\gamma' J', \gamma J) = 2C_k \left[\alpha(E_{\gamma' J'} - E_{\gamma J})\right]^{2k+1} \frac{S^{\pi k}(\gamma' J', \gamma J)}{g_{J'}}, \tag{10}$$

where $C_k = (2k+1)(k+1)/k[(2k+1)!!]^2$, and $S^{\pi k}(\gamma' J', \gamma J)$, k and $g_{J'}$ denote line strength, rank of a spherical tensor operator and statistical weight of the upper level, namely $g_{J'} = 2J' + 1$, respectively.

The largest transition rate (or probability) is electric dipole (E1) radiation. There are rules related to the parity of the transition operators. For the electric operators, parity is given by $(-1)^k$. If the parities of two levels are denoted by π and π', then

$$\boldsymbol{E}^{(k)} : \frac{\pi'}{\pi} = (-1)^k \tag{11}$$

for electric multipole transitions, where k is angular momentum of the emitted or absorbed photon. The electric dipole operator, $\boldsymbol{E}^{(1)}$, combines states of different parity.

3. Results and discussion

In this work, energies (cm^{-1}) relative to $5d6s^2\ ^2D_{3/2}$ ground state and Landé factors have been calculated for $5d6s^2$, $5d^26s$, $5d^3$, $5d6s7s$, $4f6s6p$, $5d6s6p$, $5d^26p$, and $4f5d6s$ excited levels outside core [Xe] in neutral lanthanum (La I). Some transition energies, ΔE (cm^{-1}), and lifetimes, τ (ns), for some excited levels have been also obtained for electric dipole transition (E1) between the selected $5d6snp$, $5d^2np$, np^3, ns^27p, $4f5dns$ ($n = 6, 7$), $4fnd^2$ ($n = 5, 6$), $6p7s^2$, $5d6p7s$, $5d7s7p$, $6s6p7s$, $6s7s7p$, $6p^27p$, and $6p7p^2$ configurations for odd-parity levels and the $5dns^2$, $5d^2ns$, $5dnp^2$, $6snp^2$, $4f6snp$ ($n = 6, 7$), $4f^25d$, $4f6p7s$, $4f7s7p$, $5d^3$, $6p^27s$, $6s7s^2$, $7s7p^2$, $5d6s7s$, $5d6p7p$, $6s6p7p$, and $6p7s7p$ configurations for even-parity levels outside the core [Xe] in neutral lanthanum using MCHF atomic-structure package [27]. In Table I, since data obtained for these transitions are far too extensive, just a part of the results obtained are presented to make comparison with the levels in the literature. We have also adapted the calculations related with Landé factors to Cowan's formula [1]. The lifetimes for some levels and lower lying transition energies for E1 transitions are given and compared in Table II. This table contains the lifetime calculations according to the formula (9) for $5d6s6p$, $5d^26p$, and $4f5d6s$ levels considering all possible transitions to lower levels, and the transition energies from those levels to lower levels having highest transition probabilities (or rates). Only odd-parity states are indicated by "o" superscript in Tables.

Except for some levels an agreement is seen when our results are compared with other works. Particularly, calculation results for $4f6s6p$ are in poor agreement while $4f5d6s$ are in agreement. It can be said that these cases occur due to unfilled d and, especially, f subshells. The configuration including these subshells complicates the calculations in MCHF method. But, for all levels, Landé factors are in agreement with data in NIST [5] database and Ref. [2].

TABLE I

Energies, E [cm^{-1}], and Landé factors for some excited levels in La I.

Levels			E [cm^{-1}]		Landé factor		
Configuration	Term	J	This work	Other works	This work	Other works [5]	Other works [2]
For even-parity:							
$5d6s^2$	^2D	3/2	0.000	0.000^a, 0.000^b	0.800	0.79755	–
		5/2	1066.009	1053.200^a, 1053.164^b	1.200	1.19907	–
$5d^2(^3F)6s$	^4F	3/2	2754.743	2668.200^a, 2668.188^b	0.400	0.40446	–
		5/2	3149.587	3010.010^a, 3010.002^b	1.028	1.02940	–
		7/2	3711.362	3494.580^a, 3494.526^b	1.238	1.23742	–
		9/2	4430.254	4121.610^a, 4121.572^b	1.333	1.33278	–
$5d^2(^3F)6s$	^2F	5/2	7358.505	7011.900^a, 7011.909^b	0.857	0.89830	–
		7/2	8469.856	8052.150^a, 8052.162^b	1.143	1.13469	–
$5d^2(^1D)6s$	^2D	3/2	9107.357	8446.030^a, 8446.044^b	0.800	0.93603	–
$5d^2(^3P)6s$	^4P	1/2	9209.886	7231.360^a, 7231.407^b	2.666	2.65252	–
		3/2	9524.798	7490.460^a, 7490.521^b	1.733	1.70427	–
		5/2	9400.125	7679.940^a, 7679.939^b	1.600	1.50558	–
$5d^2(^3P)6s$	^2P	1/2	9754.123	9044.210^a, 9044.214^b	0.666	0.690	–
$5d^3$	^4F	3/2	9763.552	12430.609^b	0.400	0.411	–
		5/2	10037.775	12787.404^b	1.028	1.026	–
		7/2	10608.642	13238.323^b	1.238	1.228	–
		9/2	11159.695	13747.276^b	1.333	–	–
$5d^2(^1G)6s$	^2G	7/2	11617.376	9960.960^a, 9960.904^b	0.888	0.892	–
		9/2	11808.227	9919.940^a, 9919.821^b	1.111	1.107	–
$5d^3$	^4P	1/2	14817.644	16617.30^b	2.666	–	–
		3/2	15028.325	16735.14^b	1.733	1.698	–
		5/2	15358.154	17099.38^b	1.600	–	–
$5d^3$	^2D	3/2	17567.854	18037.64^b	0.800	–	–
		5/2	18443.393	18776.62^b	1.200	–	–
$5d^3$	^2P	1/2	20417.700	20392.60^b	0.666	0.709	–
		3/2	21209.733	21037.30^b	1.333	1.316	–
$5d^3$	^2H	9/2	20437.303	18315.88^b	0.909	–	–
		11/2	20716.276	18310.92^b	1.091	0.970	–
$5d^3$	^2F	7/2	24107.610	21943.80^b	1.143	–	–
		5/2	24182.201	21969.32^b	0.857	–	–
$5d^3$	$^2D1$	5/2	28668.479	25414.63^b	1.200	–	–
$5d6s(^3D)7s$	^4D	1/2	38591.299	30019.24^b	0.000	0.000	–
		3/2	38775.919	30169.82^b	1.200	0.91	–
		5/2	39168.979	30354.28^b	1.371	1.07	–
		7/2	39854.970	31287.59^b	1.429	1.41	–
$4f6s(^3F)6p$	^4F	3/2	143927.6096	28742.34^b	0.400	0.45	–
		5/2	142794.9979	28754.96^b	1.028	0.93	–
		7/2	143231.9704	30055.05^b	1.238	1.19	–
$4f6s(^3F)6p$	^4D	1/2	156793.9584	31061.85^b	0.000	0.000	–
		3/2	156079.0208	30988.36^b	1.200	1.12	–
		5/2	154241.9952	30908.86^b	1.371	1.25	–
		7/2	152979.0659	31925.00^b	1.429	1.27	–

The transition energies obtained (except for some transitions) are in agreement with other results (in Table II). Particularly, calculation results for some $5d^26p$–$5d6s^2$, $5d6s6p$–$5d6s^2$, $5d6s6p$–$5d^26s$, and $5d^26p$–$5d^26s$ transitions are in very good agreement. But for $4f5d6s$–$5d^26s$ transition energies the agreement

TABLE I (cont.)

Levels			E [cm^{-1}]		Landé factor		
Configuration	Term	J	This work	Other works	This work	Other works [5]	Other works [2]
For odd- parity:							
$5d6s(^3D)6p$	$^4F^o$	3/2	13232.437	13260.38^b	0.400	0.52	–
		5/2	14588.443	14804.100^a, 14804.08^b	1.028	1.09	–
		7/2	15047.541	15019.550^a, 15019.51^b	1.238	1.237	–
		9/2	16147.881	16243.17^b	1.333	–	–
$5d6s(^3D)6p$	$^4D^o$	1/2	14224.056	14095.700^a, 14095.69^b	0.000	0.357	–
$5d6s(^3D)6p$	$^4D^o$	3/2	14813.862	14708.960^a, 14708.92^b	1.200	1.01	–
		5/2	15245.165	15503.670^a, 15503.64^b	1.371	1.36	–
		7/2	15820.596	16099.280^a, 16099.29^b	1.429	1.37	–
$5d^2(^3F)6p$	$^4G^o$	5/2	16418.444	17947.160^a, 17947.13^b	0.571	1.061	–
		7/2	15929.488	18603.950^a, 18603.92^b	0.984	1.051	–
		9/2	16976.127	19129.340^a, 19129.31^b	1.171	1.173	–
		11/2	17968.328	20117.400^a, 20117.38^b	1.272	1.290	–
$5d^2(^3F)6p$	$^2D^o$	3/2	16833.954	18172.390^a, 18172.35^b	0.800	0.799	0.835
		5/2	18016.456	19379.440^a, 19379.40^b	1.200	1.186	1.192
$5d6s(^3D)6p$	$^2P^o$	1/2	16992.333	25453.920^a	0.666	–	–
$5d^2(^3F)6p$	$^2F^o$	7/2	17188.287	16538.440^a	1.143	–	–
		5/2	19943.941	16856.820^a	0.857	–	–
$5d6s(^3D)6p$	$^4P^o$	1/2	17991.094	17567.49^b	2.666	2.63	–
		3/2	18613.543	17797.29^b	1.733	1.69	–
		5/2	18619.409	18157.000^a, 18156.97^b	1.600	1.175	–
$5d^2(^3F)6p$	$^4F^o$	3/2	17938.358	20083.020^a, 20082.98^b	0.400	0.724	–
		5/2	18347.598	20338.300^a, 20338.25^b	1.028	1.006	–
		7/2	18722.185	20763.310^a, 20763.21^b	1.238	1.178	–
		9/2	19578.111	21384.060^a, 21384.00^b	1.333	1.278	–
$5d^2(^3F)6p$	$^2G^o$	7/2	19427.255	21662.610^a, 21662.51^b	0.888	0.995	–
		9/2	20632.930	22285.850^a, 22285.77^b	1.111	1.13	–
$5d^2(^3F)6p$	$^4D^o$	1/2	19509.341	22246.640^a, 22246.64^b	0.000	0.04	0.025
		3/2	20728.772	22439.370^a, 22439.36^b	1.200	1.192	1.196
		5/2	20853.930	22804.260^a, 22804.25^b	1.371	1.362	1.364
		7/2	21483.213	23303.310^a, 23303.26^b	1.429	1.178	1.417
$5d^2(^3P)6p$	$^2S^o$	1/2	23052.633	23260.900^a, 23260.92^b	2.000	1.891	–
$5d^2(^3P)6p$	$^4S^o$	3/2	23917.544	24639.270^a, 24639.26^b	2.000	1.781	–
$5d^2(^3P)6p$	$^4D^o$	1/2	23843.621	23528.380^a, 23528.45^b	0.000	0.153	–
		3/2	24110.761	23704.760^a, 23704.81^b	1.200	1.133	–
		5/2	24536.547	24046.060^a, 24046.10^b	1.371	1.271	–
		7/2	25087.221	25083.420^a, 25083.36^b	1.429	1.381	1.312
$5d^2(^3P)6p$	$^2D^o$	3/2	25367.405	25950.390^a, 25950.32^b?	0.800	1.433	–
		5/2	25972.070	25218.250^a, 25218.27^b?	1.200	1.244	–
$5d^2(^3P)6p$	$^4P^o$	1/2	25957.876	25616.900^a, 25616.95^b	2.666	2.274	–
		3/2	26015.609	25643.020^a, 25643.00^b	1.733	1.59	–
		5/2	26087.066	26338.900^a, 26338.93^b	1.600	1.524	–

is much worse than with others. Also, the lifetimes for upper levels are given together with data from other works in Table II. The agreement is good except the lifetimes for some levels. We also see the differences among the other works data when we consider the results of other works. Again this can be explained by complex electronic structure with an unfilled $4f$ subshell. This subshell makes

TABLE I (cont.)

Levels			E [cm^{-1}]		Landé factor		
Configuration	Term	J	This work	Other works	This work	Other works [5]	Other works [2]
$5d^2(^1G)6p$	$^2G^o$	7/2	26403.496	27132.500^a, 27132.44^b	0.888	0.94	–
		9/2	26417.628	27619.690^a, 27619.54^b	1.111	1.12	–
$5d^2(^1D)6p$	$^2D^o$	3/2	26582.888	27968.530^a	0.800	–	–
		5/2	27417.240	28506.390^a	1.200	–	–
$5d^2(^1G)6p$	$^2H^o$	11/2	27632.141	25874.680^a	1.091	–	–
$5d^2(^3P)6p$	$^2P^o$	3/2	27562.227	27225.270^a, 27225.26^b	1.333	1.31	1.331
		1/2	27894.521	27749.050^a, 27748.97^b	0.666	0.682	–
$5d6s(^1D)6p$	$^2P^o$	1/2	28990.650	20197.380^a	0.666	–	–
		3/2	29170.163	20019.000^a	1.333	–	–
$5d6s(^3D)6p$	$^2D^o$	3/2	30643.817	15031.650^a	0.800	–	–
$4f5d(^3H)6s$	$^4H^o$	7/2	36420.346	24088.54^b	0.666	0.72	–
		9/2	36856.410	24249.00^b	0.969	0.96	–
		11/2	37454.837	24841.42^b	1.132	1.15	–
$4f5d(^3F)6s$	$^4F^o$	3/2	37552.517	24173.860^a, 24173.83^b	0.400	0.717	–
$4f5d(^3F)6s$	$^4F^o$	5/2	37854.600	24507.890^a, 24507.87^b	1.028	1.158	1.185
		7/2	38261.403	25378.460^a, 25380.27^b	1.238	1.228	1.227
		9/2	39091.197	25997.270^a, 25997.17^b	1.333	1.319	1.325
$4f5d(^1G)6s$	$^2G^o$	9/2	38416.495	23466.850^a, 23466.84^b	1.111	1.11	–
		7/2	38575.685	24409.700^a	0.888	–	–
$4f5d(^3H)6s$	$^2H^o$	11/2	40846.558	28179.07^b	1.091	1.098	–
$5d^2(^3F)7p$	$^4F^o$	3/2	44141.046	34015.76^b?	0.400	0.60	–
		5/2	44559.502	34213.53^b?	1.028	–	–
		7/2	45207.763	34988.17^b?	1.238	–	–
		9/2	44164.236	35888.45^b?	1.333	–	–
$4f5d(^3G)6s$	$^4G^o$	5/2	50458.531	27022.600^a, 27022.62^b	0.571	0.58	–
		7/2	50951.931	27455.340^a, 27455.31^b	0.984	0.976	0.991
		9/2	51521.633	28089.180^a, 28089.17^b	1.171	1.163	–
		11/2	52181.831	28743.100^a, 28743.24^b	1.272	1.27	–
$4f5d(^3D)6s$	$^4D^o$	1/2	54635.599	28893.470^a, 28893.51^b	0.000	0.018	–
		3/2	54936.293	28971.820^a, 28971.84^b?	1.200	0.884	–
		5/2	55485.755	29502.170^a, 29502.18^b?	1.371	1.263	–

^{a}Ref. [4], ^{b}Ref. [5]

the calculations very difficult. In addition, the laboratory analyses are extremely fragmentary or missing for La I. In order to cope with difficulties, we varied some parameter values in the MCHF atomic structure package. But, because of the collapse of the $4f$ orbital, the accurate calculations of wave functions in lanthanum are extremely complex. However, we have tried to present some calculations of lifetime values. We think that much larger configuration sets should be selected for more accurate lifetime values. But, in this case the computer constraints have occurred.

In conclusion, we wanted to perform the MCHF calculations for obtaining a description of La I spectrum. We reported data including valence correlation and the Breit–Pauli relativistic corrections. There is an increasing need for accurate spectroscopic data, i.e., wavelengths, radiative transition rates, oscillator strengths, branching fractions, radiative lifetimes, hyperfine structure, and isotope

TABLE II

Transition energies, ΔE [cm^{-1}], for electric dipole transitions and lifetimes, τ [ns], for upper levels in La I.

Upper level			Lower level			ΔE		τ	
Config.	Term	J	Config.	Term	J	This w.	Other w.	This w.	Other w.
$5d6s(^3D)6p$	$^4F^o$	3/2	$5d6s^2$	^2D	3/2	13232.36	–	301.5	–
$5d6s(^3D)6p$	$^4F^o$	5/2	$5d6s^2$	^2D	3/2	14588.36	–	770.68	–
$5d6s(^3D)6p$	$^4F^o$	7/2	$5d6s^2$	^2D	5/2	13981.45	–	794.09	–
$5d6s(^3D)6p$	$^4F^o$	9/2	$5d^2(^3F)6s$	^4F	9/2	11717.56	–	1974.83	–
$5d6s(^3D)6p$	$^4D^o$	1/2	$5d^2(^3F)6s$	^4F	3/2	11469.25	11427.5^a	295.18	–
$5d6s(^3D)6p$	$^4D^o$	3/2	$5d^2(^3F)6s$	^4F	3/2	12059.05	–	330.63	–
$5d6s(^3D)6p$	$^4D^o$	5/2	$5d^2(^3F)6s$	^4F	7/2	11533.74	12009.09^a	196.80	–
$5d6s(^3D)6p$	$^4D^o$	7/2	$5d^2(^3F)6s$	^4F	9/2	11390.28	11977.67^a	270.92	–
$5d6s(^3D)6p$	$^4P^o$	1/2	$5d^2(^3P)6s$	^4P	3/2	8466.25	–	733.43	–
$5d6s(^3D)6p$	$^4P^o$	3/2	$5d6s^2$	^2D	5/2	17547.43	–	218.88	–
$5d6s(^3D)6p$	$^4P^o$	5/2	$5d6s^2$	^2D	5/2	17553.30	17103.8^a	59.60	–
$5d^2(^3P)6p$	$^4D^o$	1/2	$5d^2(^3P)6s$	^4P	1/2	14633.65	16297.02^a	20.97	–
$5d^2(^3P)6p$	$^4D^o$	3/2	$5d^2(^3P)6s$	^4P	3/2	14585.88	16214.3^a	20.74	–
$5d^2(^3P)6p$	$^4D^o$	5/2	$5d^2(^3P)6s$	^4P	3/2	15011.66	16555.6^a	17.37	–
$5d^2(^3P)6p$	$^4D^o$	7/2	$5d^2(^3P)6s$	^4P	5/2	15687.01	17403.48^a	17.30	21.1(0.9)^{c1} 28.66^{c2}
$5d^2(^3P)6p$	$^2D^o$	3/2	$5d6s^2$	^2D	3/2	25367.26	24762.62^a	13.73	13.5(1.0)^e
$5d^2(^3P)6p$	$^2D^o$	5/2	$5d6s^2$	^2D	5/2	24905.92	24165.05^a	9.55	–
$5d^2(^3F)6p$	$^4D^o$	1/2	$5d6s^2$	^2D	3/2	19509.23	–	9.40	10.1(0.9)^{c1} 9.29^{c2}
$5d^2(^3F)6p$	$^4D^o$	3/2	$5d6s^2$	^2D	5/2	19662.65	–	10.31	10.2(0.5)^{c1} 9.40^{c2}
$5d^2(^3F)6p$	$^4D^o$	5/2	$5d^2(^3F)6s$	^4F	7/2	17142.47	19309.68^a 19309.724^b	9.07	10.7(1.0)^{c1} 9.70^{c2}
$5d^2(^3F)6p$	$^4D^o$	7/2	$5d^2(^3F)6s$	^4F	9/2	17052.86	19181.7^a	9.20	16.1(0.1)^{c1} 9.91^{c2}
$5d^2(^3F)6p$	$^2D^o$	3/2	$5d6s^2$	^2D	3/2	16833.86	18172.390^a 18172.35^b	21.65	17.7(1.4)^{c1} 14.13^{c2} 18(3)d 16(1)^e
$5d^2(^3F)6p$	$^2D^o$	5/2	$5d6s^2$	^2D	5/2	16950.35	18326.24^a 18326.236^b	21.56	17.2(1.0)^{c1} 13.59^{c2} 16(1.5)^e
$5d^2(^3F)6p$	$^4F^o$	3/2	$5d^2(^3F)6s$	^4F	3/2	15183.53	17414.82^a	17.05	–
$5d^2(^3F)6p$	$^4F^o$	5/2	$5d^2(^3F)6s$	^4F	5/2	15197.93	17328.29^a	21.66	–
$5d^2(^3F)6p$	$^4F^o$	7/2	$5d^2(^3F)6s$	^4F	7/2	15010.74	17268.73^a	22.23	–
$5d^2(^3F)6p$	$^4F^o$	9/2	$5d^2(^3F)6s$	^4F	9/2	15147.77	17262.45^a 17262.428^b	19.18	–
$5d^2(^3F)6p$	$^2F^o$	5/2	$5d^2(^3F)6s$	^2F	5/2	12585.36	13960.32^a	62.28	–
$5d^2(^3F)6p$	$^2F^o$	7/2	$5d6s^2$	^2D	5/2	16122.19	15485.24^a	41.55	–

shift data for lanthanide ions. The spectra of lanthanides analysis provides useful information among other things on the chemical composition of the different types of stars in astrophysics, and accurate atomic data are required in the models used for lamp design and diagnostics. In addition, the lanthanide ions can be used as a sensitive probe of crystalline structure of the salts. Consequently, we hope that the results obtained will be useful for researches in these fields.

TABLE II (cont.)

Upper level			Lower level			ΔE		τ	
Config.	Term	J	Config.	Term	J	This w.	Other w.	This w.	Other w.
$5d^2(^3F)6p$	$^4G^o$	5/2	$5d^2(^3F)6s$	^4F	3/2	13663.62	15278.96[a]	39.68	51(4)[d]
$5d^2(^3F)6p$	$^4G^o$	7/2	$5d^2(^3F)6s$	^4F	5/2	12779.83	15593.94[a]	44.89	–
$5d^2(^3F)6p$	$^4G^o$	9/2	$5d^2(^3F)6s$	^4F	7/2	13264.69	15634.76[a] 15634.784[b]	32.37	–
$5d^2(^3F)6p$	$^4G^o$	11/2	$5d^2(^3F)6s$	^4F	9/2	13538.00	15995.79[a] 15995.808[b]	36.56	–
$5d^2(^3F)6p$	$^2G^o$	7/2	$5d^2(^3F)6s$	^4F	7/2	15715.80	18168.03[a]	40.81	–
$5d^2(^3F)6p$	$^2G^o$	9/2	$5d^2(^3F)6s$	^4F	7/2	16921.47	18791.27[a]	49.09	–
$5d^2(^3P)6p$	$^4P^o$	1/2	$5d^2(^3P)6s$	^4P	3/2	16432.99	18126.44[a]	15.48	–
$5d^2(^3P)6p$	$^4P^o$	3/2	$5d^2(^3P)6s$	^4P	5/2	16615.39	17963.08[a]	14.66	–
$5d^2(^3P)6p$	$^4P^o$	5/2	$5d^2(^3P)6s$	^4P	5/2	16686.85	18658.96[a]	12.69	–
$5d^2(^3P)6p$	$^2P^o$	1/2	$5d^2(^1D)6s$	^2D	3/2	17187.55	18779.24[a]	13.73	–
$5d^2(^3P)6p$	$^2P^o$	3/2	$5d6s^2$	^2D	3/2	27562.07	27225.27[a]	23.53	17.1(0.9)[c1] 26.86[c2]
$4f5d(^3F)6s$	$^4F^o$	3/2	$5d^2(^3F)6s$	^4F	3/2	34797.58	21505.66[a]	6.04	12.5(1.5)[e]
$4f5d(^3F)6s$	$^4F^o$	5/2	$5d^2(^3F)6s$	^4F	5/2	34704.82	21497.88[a]	6.24	21.9(1.0)[c1] 16.27[c2] 14.5(1.5)[e]
$4f5d(^3F)6s$	$^4F^o$	7/2	$5d^2(^3F)6s$	^4F	7/2	34549.85	21885.75[a]	5.67	23.2(1.5)[c1] 12.40[c2]
$4f5d(^3F)6s$	$^4F^o$	9/2	$5d^2(^3F)6s$	^4F	9/2	34666.75	21875.66[a]	7.11	23.3(1.5)[c1] 12.78[c2]
$4f5d(^3H)6s$	$^4H^o$	7/2	$5d^2(^1G)6s$	^2G	7/2	24802.83	–	341.18	–
$4f5d(^3H)6s$	$^4H^o$	9/2	$5d^2(^1G)6s$	^2G	9/2	25048.04	–	375.50	–
$4f5d(^3H)6s$	$^4H^o$	11/2	$5d^2(^3F)6s$	^4F	9/2	33024.40	–	2858.77	–
$4f5d(^3G)6s$	$^4G^o$	5/2	$5d^2(^3F)6s$	^4F	5/2	47308.68	–	4.77	–
$4f5d(^3G)6s$	$^4G^o$	7/2	$5d^2(^3F)6s$	^4F	7/2	47240.32	23960.76[a]	5.06	21.6(1.6)[c1] 9.48[c2]
$4f5d(^3G)6s$	$^4G^o$	9/2	$5d^2(^3F)6s$	^4F	9/2	47091.11	–	10.93	–
$4f5d(^3G)6s$	$^4G^o$	11/2	$5d^2(^3F)6s$	^4F	9/2	47751.31	24621.49[a] 24621.668[b]	1.36	–
$4f5d(^3D)6s$	$^4D^o$	1/2	$5d^2(^3P)6s$	^4P	3/2	45425.45	–	1.22	–
$4f5d(^3D)6s$	$^4D^o$	3/2	$5d^2(^3P)6s$	^4P	3/2	45411.24	–	1.21	–
$4f5d(^3D)6s$	$^4D^o$	5/2	$5d^2(^3P)6s$	^4P	3/2	45960.70	22011.71[a]	1.01	–

[a]Ref. [4], [b]Ref. [5], [c1, c2]Ref. [2], [d]Ref. [15], [e]Ref. [17]

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