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Energies and lifetimes for highly excited levels of Lu III

Abstract

The energies and lifetimes for the $4f^{14}ns$ (n = 6-30), $4f^{14}nd$ (n = 5-30), $4f^{14}ng$ (n = 5-30), $4f^{14}nf$ (n = 5-30), and $4f^{14}np$ (n = 6-30) excited levels of doubly ionized lutetium (Lu III, Z = 71) have been obtained by using the relativistic Hartree-Fock (HFR) method. The Landé g-factors of these levels have been also calculated. In this method, configuration interaction and relativistic effects have been included in the computations combined with a least squares fitting of the Hamiltonian eigenvalues to the observed energy levels. We have compared the results with the available calculations and experiments in literature.

Key Words

Relativistic corrections; Energy levels; Lifetimes; Landé g-factors; HFR method.

INTRODUCTION

Doubly ionized lutetium (Lu III) is characterized by a simple atomic structure with a full $4f^{14}$ subshell appearing in the core and only one outer electron. The levels due to the single outer electron exhibit the properties of this sequence in that their configuration position and spin-orbit interactions are end points for the regular variation of these properties.

There is substantial spectroscopic literature concerning Lu III, though less than for the neutral or singly ionized species. The available theoretical and experimental works on energy levels and transition parameters for doubly ionized lutetium can be found in the literature[1-12]. These works were detailed in our previous work[13].

In this work, the energies, Landé g-factors, and lifetimes for highly excited levels for doubly ionized lutetium (Lu III). These calculations have been performed by using code[14] developed by Cowan for relativistic Hartree-Fock (HFR) calculations[15]. The open shell configuration structure of Lu III is similar to of La III except 4f shell in core configuration. Its ground state is $6s\ ^2S_{1/2}$, with a closed shell formed by the 14f electrons. We studied with two configuration sets. For core-valence correlation, we have only taken into account the configurations including one electron excitation from 4f subshell to other high subshells: $4f^{14}ns$ (n = 6-10), $4f^{14}np$ (n = 6-10), $4f^{14}nd$ (n = 5 - 10), $4f^{14}ng$ (n = 5 - 10), $4f^{14}nf$ (n = 5 - 10), $4f^{13}5d6p$, $4f^{13}6s6p$, $4f^{13}5d6s$, $4f^{13}6s^2$, and $4f^{13}5d^2$. For valence excitations, we have only taken into account the configurations including one electron excitation from valence to other high subshells: $4f^{14}ns$ (n = 6 - 30), $4f^{14}np$ (n = 6 - 30), $4f^{14}nd$ (n = 5 - 30), $4f^{14}ng$ (n = 5 - 30), and $4f^{14}nf$ (n = 5 - 30). These sets are denoted by A for core-valence correlation and B for valence excitations, respectively, in tables. We reported various calculations related to atomic structure (energy levels, transition energies, lifetimes, and electric dipole transitions) for Lu I, Lu II, and Lu III[13,16-19].

CALCULATION METHOD

In HFR method[15], for N electron atom of nuclear charge Z_0, the Hamiltonian is expanded as

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

in atomic units, with r_i the distance of the ith electron from the nucleus and $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$. $\zeta_i(R) = \frac{\alpha^2}{2}\frac{1}{r}\left(\frac{\partial V}{\partial r}\right)$

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.

In this method, one calculates single-configuration radial functions for a spherically symmetrised atom (center-of-gravity energy of the configuration) based on Hartree-Fock method. The radial wave functions are also used to obtain the atom's total energy (E_{av}) including approximate relativistic and correlation energy corrections. Relativistic terms in the potential function give approximate relativistic corrections to the radial functions, as well as improved relativistic energy corrections in heavy atoms. In addition, a correlation term is included to make the potential function more negative, thereby helping to bind negative ions. These radial functions are also used to calculate Coulomb integrals F^k and G^k and spin-orbit integrals ζ_{nl}. After radial functions have been obtained based on Hartree-Fock model, the 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 formula

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

If determinant wave functions are used for the atom, the total binding energy is given by

$$E = \sum_i (E_k^i + E_n^i + \sum_{j<i} E^{ij}) \quad (3)$$

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

In this method, relativistic corrections have been limited to calculations to the mass-velocity and the Darwin corrections by using the relativistic correction to total binding energy. The total binding energy can be given in by formulas (7.57), (7.58), and (7.59) in[15].

The Landé g-factor of an atomic level is related to the energy shift of the sublevels having magnetic number M by

$$\Delta E(\gamma JM) = \mu_B B g_{\gamma J} M \quad (4)$$

where B is the magnetic field intensity and μ_B is the Bohr magneton. The Landé g-factor of a level, denoted as αJ, belonging to a pure LS-coupling term is given by the formula

$$g_{\alpha LSJ} = 1 + (g_s - 1)\frac{J(J+1) - L(L+1) + S(S+1)}{2J(J+1)} \quad (5)$$

This expression is derived from vector coupling formulas by assuming a g value of unity for a pure orbital angular momentum and writing the g value for a pure electron spin (S level) as g_S[20]. A value of 2 for g_S yields the Landé formula. The Landé g-factors for energy levels are a valuable aid in the analysis of a spectrum.

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

$$\tau_j = \frac{1}{\sum_j A_{ji}}. \quad (6)$$

In the formula (6), the total transition probability, the total transition probability from a state $\gamma' J' M'$ to all states M levels of γJ is given by

$$A = \frac{64\pi^4 e^2 a_0^2 \sigma^3}{3h} \boldsymbol{S} \sum_{Mq} \begin{pmatrix} J & 1 & J' \\ -M & q & M' \end{pmatrix}^2 = \frac{64\pi^4 e^2 a_0^2 \sigma^3}{3h(2J'+1)} \boldsymbol{S} \quad (7)$$

where, $\sigma = [(E_j - E_i)/hc]$ has units of kaysers (cm^{-1}) and $\boldsymbol{S} = \left|\left\langle \gamma J \left\| \boldsymbol{P}^{(1)} \right\| \gamma' J' \right\rangle\right|^2$ is the electric dipole line strength in atomic units of $e^2a^2_0$.

RESULTS AND DISCUSSION

In this work, we have calculated the energies, Landé g-factors, and lifetimes for excited levels in Lu III (Z = 71) by using Cowan code[14] based on relativistic Hartree-Fock method[15]. We have taken into account $4f^{14}ns$ (n = 6 - 10), $4f^{14}np$ (n = 6 - 10), $4f^{14}nd$ (n = 5 - 10), $4f^{14}ng$ (n = 5 - 10), $4f^{14}nf$ (n = 5 - 10), $4f^{13}5d6p$, $4f^{13}6s6p$, $4f^{13}5d6s$, $4f^{13}6s^2$, and $4f^{13}5d^2$ configurations for calculation A, and $4f^{14}ns$ (n = 6 - 30), $4f^{14}np$ (n = 6 - 30), $4f^{14}nd$ (n = 5 - 30), $4f^{14}ng$ (n = 5 - 30), and $4f^{14}nf$ (n = 5 - 30) configurations for calculation B outside the core [Xe] in Lu III. Results obtained have been displayed in TABLE 1 and in TABLE 2 for low-lying and highly-lying excited levels. References for other comparison values are indicated below the tables with a lowercase superscript. Also, odd-parity states are indicated by the superscript "o". In calculations, the Hamiltonian's 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[21]. 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, while the spin-orbit parameters were left at their initial values. This low value of the scaling factors has been suggested by Cowan for neutral heavy elements[14,15].

TABLE 1 shows the energies, Landé g-factors, and lifetimes for $4f^{14}ns$ (n = 6-10), $4f^{14}np$ (n = 6-10), $4f^{14}nd$ (n = 5-9), $4f^{14}nf$ (n = 5-9), and $4f^{14}5g$ excited levels outside the core [Xe]. The level energies have been presented as energies (in cm^{-1}) relative to the $4f^{14}6s\ ^2S_{1/2}$ ground state. We have compared our results with previous theoretical[8-11] and

TABLE 1 : Energies, E, Landé *g*-factors, and lifetimes, τ, for low-lying levels in Lu III.

Level		E [cm^{-1}]		g-factors		τ [ns]	
Conf.	Term	This work	Other works	This work	Other works	This work	Other works
$4f^{14}6s$	$^2S_{1/2}$	0.00[A,B]	0.00[a,b,c]	2.002[A,B]	2.002[d]		
$4f^{14}5d$	$^2D_{3/2}$	5707.60[A,B]	5707.6[a]	0.800[A,B]	0.800[d]		
			2702[b]				
			5707.67[c]				
	$^2D_{5/2}$	8647.80[A,B]	8647.8[a]	1.200[A,B]	1.200[d]		
			5085[b]				
			8647.75[c]				
$4f^{14}6p$	$^2Po_{1/2}$	38400.61[A,B]	38400.61[a]	0.666[A,B]	0.666[d]	1.950[A]	1.73[c1], 2.19[c2],
			37255[b]			1.685[B]	2.54[c3], 2.23[e],
			38400.66[c]				2.1±0.2[f]
	$^2Po_{3/2}$	44705.21[A,B]	44705.21[a]	1.334[A,B]	1.334[d]	1.305[A]	1.18[c1], 1.46[c2],
			43095[b]			1.112[B]	1.66[c3], 1.47[e],
			44705.30[c]				<1.8[f]
$4f^{14}7s$	$^2S_{1/2}$	86681.21[A,B]	86681.21[a]	2.002[A,B]	2.002[d]	1.197[A]	1.167[c1], 1.135[c2],
			84312[b]			1.141[B]	1.114[c3]
			86647.41[c]				
$4f^{14}6d$	$^2D_{3/2}$	92321.60[A,B]	92321.6[a]	0.800[A,B]	0.800[d]	0.825[A]	0.857[c1], 0.953[c2],
			89363[b]			0.756[B]	1.015[c3]
			92052.42[c]				
	$^2D_{5/2}$	93107.60[A,B]	93107.6[a]	1.200[A,B]	1.200[d]	1.085[A]	0.952[c1], 1.065[c2],
			90096[b]			0.991[B]	1.136[c3]
			92812.03[c]				
$4f^{14}7p$	$^2Po_{1/2}$	100357.37[A]	100357.09[a]	0.665[A]	0.799[d]	1.941[A]	7.117[c1], 7.674[c2],
		100357.09[B]	97941[b]	0.666[B]		5.230[B]	6.892[c3]
			100554.89[c]				
	$^2Po_{3/2}$	102810.82[A,B]	102810.82[a]	1.333[A]	1.418[d]	2.247[A]	4.406[c1], 5.614[c2],
			100172[b]	1.334[B]		4.044[B]	5.947[c3]
			102887.90[c]				
$4f^{14}5f$	$^2Fo_{5/2}$	105528.56[A]	105590.6[a]	0.857[A,B]	0.889[d]	0.391[A]	–
		105590.60[B]	102653[b]			0.440[B]	
			105590.96[c]				
	$^2Fo_{7/2}$	105767.19[A]	105704.1[a]	1.143[A,B]	1.138[d]	0.408[A]	–
		105704.10[B]	102667[b]			0.477[B]	
			105704.43[c]				
$4f^{14}8s$	$^2S_{1/2}$	119784.75[A,B]	119784.75[a]	1.998[A]	2.002[d]	1.568[A]	–
			116865[b]	2.002[B]		1.753[B]	
			119790.11[c]				
$4f^{14}7d$	$^2D_{3/2}$	122622.49[A]	122622.5[a]	0.815[A]	0.800[d]	1.788[A]	–
		122622.50[B]	119520[b]	0.800[B]		1.567[B]	
			122534.87[c]				
	$^2D_{5/2}$	122981.00[A,B]	122981.0[a]	1.201[A]	1.200[d]	2.033[A]	–
			119866[b]	1.200[B]		1.912[B]	
			122882.95[c]				
$4f^{14}8p$	$^2Po_{1/2}$	125782.70[A]	123423[b]	0.666[A,B]	–	8.902[A]	–
		125654.50[B]	126452.72[c]			12.230[B]	
	$^2Po_{3/2}$	126776.60[A]	124525[b]	1.334[A,B]	–	8.181[A]	–
		126653.20[B]	127593.11[c]			11.090[B]	

Level		E [cm^{-1}]		g-factors		τ [ns]	
Conf.	Term	This work	Other works	This work	Other works	This work	Other works
$4f^{14}6f$	$^2F^o_{5/2}$	128923.36^A	129053.2^a	0.857^{A,B}	0.858^d	0.648^A	–
		129053.20^B	125431^b			0.791^B	
			128623.76^c				
	$^2F^o_{7/2}$	128929.62^A	128799.8^a	1.143^{A,B}	1.143^d	0.688^A	–
		128799.80^B	125442^b			0.731^B	
			128684.78^c				
$4f^{14}5g$	$^2G_{7/2}$	129105.40^{A,B}	129105.4^a	0.906^A	0.889^d	2.489^A	–
				0.889^B		2.699^B	
	$^2G_{9/2}$	129106.30^{A,B}	129106.3^a	1.112^A	1.111^d	2.485^A	–
				1.111^B		2.737^B	
$4f^{14}9s$	$^2S_{1/2}$	136209.89^A	136209.86^a	1.922^A	2.002^d	1.614^A	–
		136209.86^B	136220.67^c	2.002^B		2.650^B	
$4f^{14}8d$	$^2D_{3/2}$	138227.88^A	137770.38^c	0.844^A	–	1.133^A	–
		137774.10^B		0.800^B		2.741^B	
	$^2D_{5/2}$	138525.69^A	137961.33^c	1.196^A	–	1.081^A	–
		137951.90^B		1.200^B		3.172^B	
$4f^{14}9p$	$^2P^o_{1/2}$	138951.40^A	139926.58^c	0.666^{A,B}	–	17.250^A	–
		138903.50^B				22.990^B	
	$^2P^o_{3/2}$	139520.90^A	140574.83^c	1.334^{A,B}	–	16.850^A	–
		139473.50^B				22.400^B	
$4f^{14}7f$	$^2F^o_{5/2}$	141069.62^A	141069.6^a	0.857^{A,B}	0.857^d	1.052^A	–
		141069.60^B	137774^b			1.193^B	
			141067.76^c				
	$^2F^o_{7/2}$	141092.17^A	141092.2^a	1.143^{A,B}	1.143^d	1.109^A	–
		141092.20^B	137781^b			1.266^B	
			141103.99^c				
$4f^{14}10s$	$^2S_{1/2}$	145587.30^{A,B}	145587.3^a	2.002^{A,B}	1.998^d	4.050^A	–
			145591.37^c			3.882^B	
$4f^{14}9d$	$^2D_{3/2}$	146495.00^A	146546.53^c	0.800^{A,B}	–	3.508^A	–
		146432.70^B				4.365^B	
	$^2D_{5/2}$	146559.00^A	146663.29^c	1.200^{A,B}	–	2.651^A	–
		146540.50^B				4.941^B	
$4f^{14}10p$	$^2P^o_{1/2}$	146758.80^A	147867.11^c	0.666^{A,B}	–	26.570^A	–
		146734.30^B				37.470^B	
	$^2P^o_{3/2}$	147114.90^A	148268.31^c	1.334^{A,B}	–	27.010^A	–
		147090.60^B				38.210^B	
$4f^{14}8f$	$^2F^o_{5/2}$	148513.81^A	148513.8^a	0.857^{A,B}	0.857^d	1.599^A	–
		148513.80^B	145198^b			1.817^B	
			148541.34^c				
	$^2F^o_{7/2}$	148529.99^A	148530.0^a	1.143^{A,B}	1.143^d	1.679^A	–
		148530.00^B	145204^b			1.920^B	
			148565.59^c				
$4f^{14}9f$	$^2F^o_{5/2}$	153343.60^{A,B}	153343.6^a	0.857^{A,B}	0.857^d	2.263^A	–
			153376.59^c			2.640^B	
	$^2F^o_{7/2}$	153354.50^A	153354.5^a	1.143^{A,B}	1.143^d	2.370^A	–
		153354.40^B	153393.05^c			2.781^B	

^{a}Ref.[21], ^{b}Ref.[9], $^{c, c1, c2, c3}$Ref.[8], ^{d}Ref.[10], ^{e}Ref.[11], ^{f}Ref.[12].

TABLE 2 : New energies, E, Landé g-factors, and lifetimes, τ, for highly excited levels in Lu III.

Level		E [cm^{-1}]	g-factors	τ [ns]	Level		E [cm^{-1}]	g-factors	τ [ns]
Conf.	Term	This work	This work	This work	Conf.	Term	This work	This work	This work
$4f^{14}6g$	$^2G_{7/2}$	141122.50[A]	0.889[A,B]	4.55[A]	$4f^{14}14s$	$^2S_{1/2}$	159817.70[B]	2.002[B]	12.34[B]
		141121.90[B]		4.83[B]	$4f^{14}13d$	$^2D_{3/2}$	160055.40[B]	0.800[B]	15.58[B]
	$^2G_{9/2}$	141123.10[A]	1.111[A,B]	4.54[A]		$^2D_{5/2}$	160081.40[B]	1.200[B]	17.00[B]
		141122.80[B]		4.75[B]	$4f^{14}12f$	$^2Fo_{5/2}$	160496.70[B]	0.857[B]	6.67[B]
$4f^{14}7g$	$^2G_{7/2}$	148454.60[A]	0.893[A]	7.20[A]		$^2Fo_{7/2}$	160499.90[B]	1.143[B]	7.00[B]
		148454.50[B]	0.889[B]	7.48[B]	$4f^{14}11g$	$^2G_{7/2}$	160540.60[B]	0.889[B]	27.71[B]
	$^2G_{9/2}$	148480.80[A]	1.111[A,B]	1.52[A]		$^2G_{9/2}$	160540.60[B]	1.111[B]	27.66[B]
		148454.90[B]		7.43[B]	$4f^{14}15p$	$^2Po_{1/2}$	160721.70[B]	0.666[B]	182.40[B]
$4f^{14}10d$	$^2D_{3/2}$	151357.08[A]	0.800[A,B]	4.59[A]		$^2Po_{3/2}$	160791.40[B]	1.334[B]	191.10[B]
		151895.40[B]		6.49[B]	$4f^{14}15s$	$^2S_{1/2}$	161295.80[B]	2.002[B]	14.72[B]
	$^2D_{5/2}$	151395.12[A]	1.200[A,B]	4.25[A]	$4f^{14}16p$	$^2Po_{1/2}$	161775.40[B]	0.666[B]	231.00[B]
		151965.90[B]		7.24[B]		$^2Po_{3/2}$	161830.20[B]	1.334[B]	242.10[B]
$4f^{14}11s$	$^2S_{1/2}$	151261.20[B]	2.002[B]	5.62[B]	$4f^{1414}d$	$^2D_{3/2}$	161477.90[B]	0.800[B]	19.26[B]
$4f^{14}11p$	$^2Po_{1/2}$	151750.00[B]	0.666[B]	55.60[B]		$^2D_{5/2}$	161497.70[B]	1.200[B]	20.92[B]
	$^2Po_{3/2}$	151987.60[B]	1.334[B]	57.70[B]	$4f^{14}13f$	$^2Fo_{5/2}$	161816.10[B]	0.857[B]	8.60[B]
$4f^{14}8g$	$^2G_{7/2}$	153214.40[A]	0.889[A,B]	10.83[A]		$^2Fo_{7/2}$	161818.50[B]	1.143[B]	9.02[B]
		153214.30[B]		11.05[B]	$4f^{14}12g$	$^2G_{7/2}$	161849.00[B]	0.889[B]	35.75[B]
	$^2G_{9/2}$	153215.20[A]	1.111[A,B]	10.84[A]		$^2G_{9/2}$	161849.00[B]	1.111[B]	35.69[B]
		153214.80[B]		11.01[B]	$4f^{14}16s$	$^2S_{1/2}$	162438.10[B]	2.002[B]	16.58[B]
$4f^{14}12s$	$^2S_{1/2}$	155127.30[B]	2.002[B]	7.635[B]	$4f^{14}15d$	$^2D_{3/2}$	162581.20[B]	0.800[B]	22.73[B]
$4f^{14}12p$	$^2Po_{1/2}$	155157.20[B]	0.666[B]	78.41[B]		$^2D_{5/2}$	162596.70[B]	1.200[B]	24.57[B]
	$^2Po_{3/2}$	155323.40[B]	1.334[B]	82.04[B]	$4f^{14}17p$	$^2Po_{1/2}$	162595.90[B]	0.666[B]	287.70[B]
$4f^{14}11d$	$^2D_{3/2}$	155568.10[B]	0.800[B]	9.130[B]		$^2Po_{3/2}$	162639.70[B]	1.334[B]	301.60[B]
	$^2D_{5/2}$	155616.60[B]	1.200[B]	10.10[B]	$4f^{14}14f$	$^2Fo_{5/2}$	162846.30[B]	0.857[B]	10.88[B]
$4f^{14}10f$	$^2Fo_{5/2}$	156411.10[A]	0.857[A,B]	3.23[A]		$^2Fo_{7/2}$	162848.10[B]	1.143[B]	11.40[B]
		156390.90[B]		3.73[B]	$4f^{14}13g$	$^2G_{7/2}$	162871.00[B]	0.889[B]	45.19[B]
	$^2Fo_{7/2}$	156417.40[A]	1.143[A,B]	3.38[A]		$^2G_{9/2}$	162871.00[B]	1.111[B]	45.12[B]
		156396.20[B]		3.93[B]	$4f^{14}18p$	$^2Po_{1/2}$	163264.10[B]	0.666[B]	352.50[B]
$4f^{14}9g$	$^2G_{7/2}$	156476.30[A]	0.889[A,B]	15.07[A]		$^2Po_{3/2}$	163299.60[B]	1.334[B]	369.40[B]
		156476.70[B]		15.66[B]	$4f^{14}17s$	$^2S_{1/2}$	163333.60[B]	2.002[B]	17.72[B]
	$^2G_{9/2}$	156477.10[A]	1.111[A,B]	15.20[A]	$4f^{14}16d$	$^2D_{3/2}$	163443.20[B]	0.800[B]	25.79[B]
		156476.70[B]		15.62[B]		$^2D_{5/2}$	163455.40[B]	1.200[B]	27.75[B]
$4f^{14}13p$	$^2Po_{1/2}$	157582.40[B]	0.666[B]	106.60[B]	$4f^{14}15f$	$^2Fo_{5/2}$	163652.70[B]	0.857[B]	13.54[B]
	$^2Po_{3/2}$	157703.30[B]	1.334[B]	111.70[B]		$^2Fo_{7/2}$	163654.10[B]	1.143[B]	14.19[B]
$4f^{14}13s$	$^2S_{1/2}$	157844.10[B]	2.002[B]	9.91[B]	$4f^{14}14g$	$^2G_{7/2}$	163673.60[B]	0.889[B]	56.32[B]
$4f^{14}12d$	$^2D_{3/2}$	158161.40[B]	0.800[B]	12.15[B]		$^2G_{9/2}$	163673.60[B]	1.111[B]	56.24[B]
	$^2D_{5/2}$	158196.40[B]	1.200[B]	13.32[B]	$4f^{14}19p$	$^2Po_{1/2}$	163818.90[B]	0.666[B]	426.70[B]
$4f^{14}11f$	$^2Fo_{5/2}$	158751.60[B]	0.857[B]	5.06[B]		$^2Po_{3/2}$	163848.20[B]	1.334[B]	447.30[B]
	$^2Fo_{7/2}$	158755.50[B]	1.143[B]	5.31[B]	$4f^{14}18s$	$^2S_{1/2}$	164062.90[B]	2.002[B]	17.46[B]
$4f^{14}10g$	$^2G_{7/2}$	158812.95[A]	0.889[A,B]	7.29[A]	$4f^{14}17d$	$^2D_{3/2}$	164151.60[B]	0.800[B]	27.33[B]
		158813.30[B]		21.06[B]		$^2D_{5/2}$	164161.60[B]	1.200[B]	29.21[B]
	$^2G_{9/2}$	158813.44[A]	1.111[A,B]	7.53[A]	$4f^{14}20p$	$^2Po_{1/2}$	164270.90[B]	0.666[B]	511.00[B]
		158813.30[B]		21.01[B]		$^2Po_{3/2}$	164295.30[B]	1.334[B]	535.60[B]
$4f^{14}14p$	$^2Po_{1/2}$	159373.10[B]	0.666[B]	141.10[B]	$4f^{14}16f$	$^2Fo_{5/2}$	164313.80[B]	0.857[B]	16.60[B]
	$^2Po_{3/2}$	159463.70[B]	1.334[B]	147.80[B]		$^2Fo_{7/2}$	164314.90[B]	1.143[B]	17.38[B]

Level		E [cm^{-1}]	g-factors	τ [ns]	Level		E [cm^{-1}]	g-factors	τ [ns]
Conf.	Term	This work	This work	This work	Conf.	Term	This work	This work	This work
$4f^{14}15g$	$^2G_{7/2}$	164333.40[B]	0.889[B]	68.86[B]	$4f^{14}23s$	$^2S_{1/2}$	166162.90[B]	2.002[B]	9.89[B]
	$^2G_{9/2}$	164333.40[B]	1.111[B]	68.77[B]	$4f^{14}28p$	$^2P^o_{1/2}$	166169.90[B]	0.666[B]	1609[B]
$4f^{14}19s$	$^2S_{1/2}$	164646.70[B]	2.002[B]	16.78[B]		$^2P^o_{3/2}$	166177.60[B]	1.334[B]	1687[B]
$4f^{14}21p$	$^2P^o_{1/2}$	164654.50[B]	0.666[B]	605.60[B]	$4f^{14}22d$	$^2D_{3/2}$	166196.20[B]	0.800[B]	20.96[B]
	$^2P^o_{3/2}$	164675.00[B]	1.334[B]	634.80[B]		$^2D_{5/2}$	166200.50[B]	1.200[B]	21.68[B]
$4f^{14}18d$	$^2D_{3/2}$	164723.10[B]	0.800[B]	28.02[B]	$4f^{14}21f$	$^2F^o_{5/2}$	166253.40[B]	0.857[B]	38.66[B]
	$^2D_{5/2}$	164731.30[B]	1.200[B]	29.75[B]		$^2F^o_{7/2}$	166253.70[B]	1.143[B]	40.41[B]
$4f^{14}17f$	$^2F^o_{5/2}$	164860.40[B]	0.857[B]	20.07[B]	$4f^{14}29p$	$^2P^o_{1/2}$	166281.60[B]	0.666[B]	1810[B]
	$^2F^o_{7/2}$	164861.40[B]	1.143[B]	21.01[B]		$^2P^o_{3/2}$	166288.40[B]	1.334[B]	1896[B]
$4f^{14}16g$	$^2G_{7/2}$	164876.70[B]	0.889[B]	83.09[B]	$4f^{14}24s$	$^2S_{1/2}$	166395.70[B]	2.002[B]	9.00[B]
	$^2G_{9/2}$	164876.70[B]	1.111[B]	82.98[B]	$4f^{14}30p$	$^2P^o_{1/2}$	166422.40[B]	0.666[B]	2021[B]
$4f^{14}17g$	$^2G_{7/2}$	164904.40[B]	0.889[B]	111.40[B]		$^2P^o_{3/2}$	166428.60[B]	1.334[B]	2118[B]
	$^2G_{9/2}$	164904.40[B]	1.111[B]	111.20[B]	$4f^{14}23d$	$^2D_{3/2}$	166431.80[B]	0.800[B]	19.32[B]
$4f^{14}22p$	$^2P^o_{1/2}$	164954.00[B]	0.666[B]	711.80[B]		$^2D_{5/2}$	166435.30[B]	1.200[B]	19.91[B]
	$^2P^o_{3/2}$	164971.40[B]	1.334[B]	746.00[B]	$4f^{14}22f$	$^2F^o_{5/2}$	166498.50[B]	0.857[B]	44.64[B]
$4f^{14}20s$	$^2S_{1/2}$	165117.10[B]	2.002[B]	15.89[B]		$^2F^o_{7/2}$	166498.90[B]	1.143[B]	46.66[B]
$4f^{14}19d$	$^2D_{3/2}$	165182.50[B]	0.800[B]	28.09[B]	$4f^{14}21g$	$^2G_{7/2}$	166505.30[B]	0.889[B]	185.70[B]
	$^2D_{5/2}$	165189.30[B]	1.200[B]	29.65[B]		$^2G_{9/2}$	166505.30[B]	1.111[B]	185.50[B]
$4f^{14}23p$	$^2P^o_{1/2}$	165231.00[B]	0.666[B]	829.00[B]	$4f^{14}25s$	$^2S_{1/2}$	166597.80[B]	2.002[B]	7.82[B]
	$^2P^o_{3/2}$	165246.00[B]	1.334[B]	868.80[B]	$4f^{14}24d$	$^2D_{3/2}$	166622.60[B]	0.800[B]	17.35[B]
$4f^{14}18f$	$^2F^o_{5/2}$	165302.10[B]	0.857[B]	23.22[B]		$^2D_{5/2}$	166625.60[B]	1.200[B]	17.81[B]
	$^2F^o_{7/2}$	165303.10[B]	1.143[B]	24.25[B]	$4f^{14}23f$	$^2F^o_{5/2}$	166679.00[B]	0.857[B]	51.55[B]
$4f^{14}18g$	$^2G_{7/2}$	165337.70[B]	0.889[B]	130.30[B]		$^2F^o_{7/2}$	166679.30[B]	1.143[B]	53.89[B]
	$^2G_{9/2}$	165337.70[B]	1.111[B]	130.10[B]	$4f^{14}26s$	$^2S_{1/2}$	166807.30[B]	2.002[B]	5.93[B]
$4f^{14}24p$	$^2P^o_{1/2}$	165481.30[B]	0.666[B]	958.10[B]	$4f^{14}22g$	$^2G_{7/2}$	166684.40[B]	0.889[B]	216.20[B]
	$^2P^o_{3/2}$	165494.20[B]	1.334[B]	1004[B]		$^2G_{9/2}$	166684.40[B]	1.111[B]	215.90[B]
$4f^{14}21s$	$^2S_{1/2}$	165519.10[B]	2.002[B]	14.26[B]	$4f^{14}25d$	$^2D_{3/2}$	166818.70[B]	0.800[B]	13.87[B]
$4f^{14}20d$	$^2D_{3/2}$	165574.40[B]	0.800[B]	26.80[B]		$^2D_{5/2}$	166821.50[B]	1.200[B]	14.17[B]
	$^2D_{5/2}$	165580.20[B]	1.200[B]	28.09[B]	$4f^{14}24f$	$^2F^o_{5/2}$	166842.30[B]	0.857[B]	58.94[B]
$4f^{14}19f$	$^2F^o_{5/2}$	165678.20[B]	0.857[B]	27.29[B]		$^2F^o_{7/2}$	166842.60[B]	1.143[B]	61.61[B]
	$^2F^o_{7/2}$	165678.90[B]	1.143[B]	28.49[B]	$4f^{14}23g$	$^2G_{7/2}$	166851.40[B]	0.889[B]	247.40[B]
$4f^{14}25p$	$^2P^o_{1/2}$	165666.10[B]	0.666[B]	1101.0[B]		$^2G_{9/2}$	166851.40[B]	1.111[B]	247.00[B]
	$^2P^o_{3/2}$	165677.30[B]	1.334[B]	1154.0[B]	$4f^{14}27s$	$^2S_{1/2}$	166986.20[B]	2.002[B]	4.81[B]
$4f^{14}26p$	$^2P^o_{1/2}$	165824.70[B]	0.666[B]	1258.0[B]	$4f^{14}26d$	$^2D_{3/2}$	167001.60[B]	0.800[B]	11.34[B]
	$^2P^o_{3/2}$	165834.60[B]	1.334[B]	1319.0[B]		$^2D_{5/2}$	167003.80[B]	1.200[B]	11.55[B]
$4f^{14}22s$	$^2S_{1/2}$	165852.40[B]	2.002[B]	12.37[B]	$4f^{14}25f$	$^2F^o_{5/2}$	167010.40[B]	0.857[B]	66.84[B]
$4f^{14}19g$	$^2G_{7/2}$	165872.50[B]	0.889[B]	144.80[B]		$^2F^o_{7/2}$	167010.80[B]	1.143[B]	69.86[B]
	$^2G_{9/2}$	165872.50[B]	1.111[B]	144.60[B]	$4f^{14}24g$	$^2G_{7/2}$	167021.70[B]	0.889[B]	278.70[B]
$4f^{14}21d$	$^2D_{3/2}$	165891.50[B]	0.800[B]	24.81[B]		$^2G_{9/2}$	167021.70[B]	1.111[B]	278.40[B]
	$^2D_{5/2}$	165896.30[B]	1.200[B]	25.84[B]	$4f^{14}28s$	$^2S_{1/2}$	167126.00[B]	2.002[B]	4.50[B]
$4f^{14}20f$	$^2F^o_{5/2}$	165973.90[B]	0.857[B]	33.06[B]	$4f^{14}27d$	$^2D_{3/2}$	167157.60[B]	0.800[B]	10.28[B]
	$^2F^o_{7/2}$	165974.60[B]	1.143[B]	34.56[B]		$^2D_{5/2}$	167159.60[B]	1.200[B]	10.45[B]
$4f^{14}27p$	$^2P^o_{1/2}$	165989.80[B]	0.666[B]	1428.0[B]	$4f^{14}26f$	$^2F^o_{5/2}$	167186.90[B]	0.857[B]	75.21[B]
	$^2P^o_{3/2}$	165998.50[B]	1.334[B]	1496.0[B]		$^2F^o_{7/2}$	167187.20[B]	1.143[B]	78.59[B]
$4f^{14}20g$	$^2G_{7/2}$	166129.70[B]	0.889[B]	169.20[B]	$4f^{14}25g$	$^2G_{7/2}$	167194.60[B]	0.889[B]	309.4[B]
	$^2G_{9/2}$	166129.70[B]	1.111[B]	168.90[B]		$^2G_{9/2}$	167194.60[B]	1.111[B]	309.0[B]

Level		E [cm^{-1}]	g-factors	τ [ns]	Level		E [cm^{-1}]	g-factors	τ [ns]
Conf.	Term	This work	This work	This work	Conf.	Term	This work	This work	This work
$4f^{14}29s$	$^2S_{1/2}$	167212.30[B]	2.002[B]	4.49[B]	$4f^{14}28f$	$^2Fo_{5/2}$	167425.80[B]	0.857[B]	94.45[B]
$4f^{14}28d$	$^2D_{3/2}$	167243.10[B]	0.800[B]	10.07[B]		$^2Fo_{7/2}$	167426.10[B]	1.143[B]	98.68[B]
	$^2D_{5/2}$	167244.90[B]	1.200[B]	10.22[B]	$4f^{14}28g$	$^2G_{7/2}$	167465.00[B]	0.889[B]	443.90[B]
$4f^{14}27f$	$^2Fo_{5/2}$	167291.30[B]	0.857[B]	84.64[B]		$^2G_{9/2}$	167465.00[B]	1.111[B]	443.30[B]
	$^2Fo_{7/2}$	167291.70[B]	1.143[B]	88.45[B]	$4f^{14}29f$	$^2Fo_{5/2}$	167471.50[B]	0.857[B]	105.80[B]
$4f^{14}26g$	$^2G_{7/2}$	167293.40[B]	0.889[B]	350.40[B]		$^2Fo_{7/2}$	167471.80[B]	1.143[B]	110.50[B]
	$^2G_{9/2}$	167293.40[B]	1.111[B]	350.00[B]	$4f^{14}29g$	$^2G_{7/2}$	167505.50[B]	0.889[B]	500.80[B]
$4f^{14}30s$	$^2S_{1/2}$	167328.00[B]	2.002[B]	4.05[B]		$^2G_{9/2}$	167505.50[B]	1.111[B]	500.20[B]
$4f^{14}29d$	$^2D_{3/2}$	167363.00[B]	0.800[B]	9.10[B]	$4f^{14}30f$	$^2Fo_{5/2}$	167504.50[B]	0.857[B]	118.00[B]
	$^2D_{5/2}$	167364.80[B]	1.200[B]	9.22[B]		$^2Fo_{7/2}$	167504.90[B]	1.143[B]	123.30[B]
$4f^{14}30d$	$^2D_{3/2}$	167389.90[B]	0.800[B]	33.23[B]	$4f^{14}30g$	$^2G_{7/2}$	167670.00[B]	0.889[B]	535.80[B]
	$^2D_{5/2}$	167391.40[B]	1.200[B]	33.81[B]		$^2G_{9/2}$	167670.00[B]	1.111[B]	535.20[B]
$4f^{14}27g$	$^2G_{7/2}$	167423.10[B]	0.889[B]	388.60[B]					
	$^2G_{9/2}$	167423.10[B]	1.111[B]	388.10[B]					

experimental[12,21] results. Most of our energy results are in good agreement with others. Moreover, we have calculated $[|E_{\text{this work}} - E_{\text{other works}}|/E_{\text{this work}}] \times 100$, the differences in per cent, for the accuracy of our results. There is very good agreement between our energies from the calculations obtained according to the B configuration set and other works[21]. In calculation A, differences (%) between our results and other experimental works[21] have been found in the 0.00–0.10 range for the energies of $4f^{14}$ns (n = 6-10), $4f^{14}$np (n = 6, 7), $4f^{14}$nd (n = 5 - 7), $4f^{14}$nf (n = 5 - 9), and $4f^{14}5g$ excited levels. When the differences (%) between our results and other theoretical results[8] are investigated, the differences in energies are generally in range of 0.00-0.80. For energies of $4f^{14}$np (n = 8-10) and $4f^{14}$nd (n = 8, 9) excited levels, there is very little discrepancy. The differences (%) between our results and other theoretical results[8] (indicated by the superscript c in TABLE 1) are in range of 0.03-0.80. There are only theoretical results[8,9] for these levels. The results obtained for levels need to experimental results because of fitting procedure in HFR method. However, we can say that our results for these levels are good. Because there are excellent agreement for other levels when compared with available experimental works. The Landé *g*-factor results are also in good agreement with[10]. For the Landé *g*-factor of $4f^{14}7p$ level the agreement is somewhat poor whereas the agreement for energy of $4f^{14}7p$ level is good.

In TABLE 1, we have also presented the lifetimes for $4f^{14}$ns (n = 7 - 10), $4f^{14}$np (n = 6 - 10), $4f^{14}$nd (n = 6 - 9), $4f^{14}$nf (n = 5 - 9), and $4f^{14}5g$ excited levels of Lu III. These lifetimes were calculated using formula (6), considering all possible transitions from the listed levels to lower ones. Only lifetime results of the $4f^{14}$np (n = 6, 7), $4f^{14}7s$ and $4f^{14}6d$ levels are compared with experimental[12] and theoretical[8,11] results. The lifetime results in[8] were used for comparing with our results after calculated using formula (6) from transition probabilities. The lifetimes obtained from the calculation A including core correlation are in agreement with other works. But lifetime of $4f^{14}7p$ level obtained from the calculation B is better. Moreover, new energies, Landé g-factors and lifetimes for $4f^{14}$ns (n = 11 - 30), $4f^{14}$np (n = 11 - 30), $4f^{14}$nd (n = 10 - 30), $4f^{14}$nf (n = 10 - 30), and $4f^{14}$ng (n = 6-30) levels of Lu III are presented in TABLE 2. Our new energy levels, Landé *g*-factors and lifetimes are reliable since the results in presented TABLE 1 is in excellent agreement with other works. In addition, we have calculated too much result for $4f^{13}5d6p$, $4f^{13}6s6p$, $4f^{13}5d6s$, $4f^{13}6s^2$, and $4f^{13}5d^2$ levels. In this paper, we have not presented results of these levels. Because there are not yet theoretical and experimental results for these levels for comparing. So, the accuracy of these levels belong to configurations of the type $4f^{13}nln'l'$ might be completely different from the one obtained for $4f^{14}nl$ configurations. One-electron spectrum is superimposed on the complex three-electron spectrum arising from the excitation of an electron out of the 4f shell.

In conclusion, the main purpose of this paper was to perform HFR calculations for highly-excited levels of the Lu III spectrum. Accurate atomic structure data is an essential ingredient for a wide range of research fields. Areas from plasma research applications in nuclear fusion to lighting research, as well as astrophysics and cosmology, depend on such data. We have here reported new data including valence and core correlation effects and relativistic corrections in Lu III. The energy data and Landé *g*-factors presented for Lu III in this work can be useful to investigations for some radiative parameters. Consequently, we hope that our results, especially new results, obtained using the HFR method will be useful for research fields and technological applications, and other works in the future for Lu III spectra.

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