

# Relativistic many-body calculation of energies, transition rates, lifetimes, and multipole polarizabilities in Cs-like La III

U. I. Safronova<sup>1,2</sup> and M. S. Safronova<sup>3,4</sup><sup>1</sup>*Physics Department, University of Nevada, Reno, Nevada 89557, USA*<sup>2</sup>*Department of Physics, University of Notre Dame, Notre Dame, Indiana 46556, USA*<sup>3</sup>*Department of Physics and Astronomy, 217 Sharp Laboratory, University of Delaware, Newark, Delaware 19716, USA*<sup>4</sup>*Joint Quantum Institute, National Institute of Standards and Technology and University of Maryland, College Park, Maryland 20742, USA*

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Excitation energies of the [Xe]*nd* ( $n = 5-9$ ), [Xe]*ns* ( $n = 6-10$ ), [Xe]*np* ( $n = 6-9$ ), [Xe]*nf* ( $n = 4-8$ ), and [Xe]*ng* ( $n = 5-8$ ) states in La III, where [Xe] =  $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6 4d^{10} 5s^2 5p^6$ , are evaluated. Electric dipole matrix elements for the allowed transitions between the low-lying [Xe]*nd*, [Xe]*ns*, [Xe]*np*, [Xe]*nf*, and [Xe]*ng* states in the La III ion are calculated using the high-precision relativistic all-order method where all single, double, and partial triple excitations of the Dirac-Fock wave functions are included to all orders of perturbation theory. Recommended values are provided for a large number of electric dipole matrix elements, oscillator strengths, transition rates, and lifetimes. Scalar and tensor polarizabilities of the states listed above are evaluated. The uncertainties of the recommended values are estimated. Electric quadrupole and magnetic dipole matrix elements are calculated to determine lifetimes of the  $5d_{5/2}$  and  $6s$  metastable levels. The ground-state  $E1$ ,  $E2$ , and  $E3$  static polarizabilities are calculated. This work provides recommended values critically evaluated for their accuracy for a number of La III atomic properties for use in planning and analysis of various experiments as well as theoretical modeling.

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## I. INTRODUCTION

Transition energies (ionization potentials and excitation energies) for doubly ionized lanthanum,  $\text{La}^{2+}$ , have been studied experimentally for almost 85 years. To the best of our knowledge, the first paper with results for doublet splitting of  $\text{La}^{2+}$  was published in 1929 by Gibbs and White [1]. Some years later, Gibbs and Schoepfle [2] extended both the  $ns\ ^2S$  and  $nd\ ^2D$  series of terms to six members, located one more pair of  $^2P$  terms, and tentatively determined some of the  $^2F$  and  $^2G$  terms. The NIST database [3] includes 42 levels based on the NIST compilation by Martin *et al.* [4].

Dipole transition probabilities, oscillator strengths, lifetimes, and branching ratios for the  $\text{La}^{2+}$  ion were calculated by Lindgård and Nielsen [5] using numerical Coulomb approximation. Migdalek and Baylis [6] presented theoretical values of the  $6s$ - $6p$  oscillator strengths in  $\text{La}^{2+}$  using the single-configuration relativistic Hartree-Fock method. Model potential calculations were performed by Migdalek and Wyrozumska [7] in order to investigate the influence of valence-core electron exchange on oscillator strengths in the Cs isoelectronic sequence. The relativistic Hartree-Fock (HFR) technique described by Cowan [8] with core-polarization effects incorporated by Biémont *et al.* [9] was used to evaluate oscillator strengths in the  $\text{La}^{2+}$  ion. Authors emphasized that radiative lifetime measurements [10] performed with time-resolved laser spectroscopy for the  $6p_{1/2}$  and  $6p_{3/2}$  levels of  $\text{La}^{2+}$  provide a unique opportunity for testing the adequacy of the relativistic Hartree-Fock approach for atomic structure calculations in this ion [9]. Biémont and Quinet [11] presented an overview of the recent developments concerning the spectroscopic properties of lanthanide atoms and ions. Authors underlined that lanthanide elements are important in astrophysics in relation to nucleosynthesis and star formation. However, their detection in the stellar spectra was frequently

hindered by the fact that they appear under the form of many medium or weak intensity lines which were blended with contributions originating from the most abundant elements, particularly those of the iron group [11]. Landé  $g$  factors were calculated by Quinet and Biémont in [12] for energy levels of doubly ionized lanthanides. Configuration interaction and relativistic effects were included in the computations using the HFR technique combined with a least-squares fitting of the Hamiltonian eigenvalues to the observed energy levels [12]. Using the HFR method developed by Cowan [8], Karaçoban and Özdemir [13] calculated the energy levels, Landé  $g$  factors, and lifetimes for excited levels of doubly ionized lanthanum.

The relativistic coupled-cluster method was applied by Eliav *et al.* [14] to the calculation of the transition energies of lanthanum. Numerical results were presented for the  $5d$ ,  $4f$ ,  $6s$ , and  $6p$  levels.

None of the previous studies listed above, except for the relativistic coupled-cluster calculations of energies for the seven levels in  $\text{La}^{2+}$  [14], were carried out by high-precision *ab initio* methods.

In the present work, the relativistic high-precision all-order (linearized coupled-cluster) method is used to calculate atomic properties of doubly ionized lanthanum for the first 42 excited  $ns$ ,  $np$ ,  $nd$ ,  $nf$ , and  $ng$  states. The reduced electric dipole matrix elements, line strengths, oscillator strengths, and transition rates are determined for allowed transitions between these levels. The  $M1\ 5d_{3/2}$ - $5d_{5/2}$ ,  $5d_{3/2}$ - $6s$  and  $E2\ 5d_{3/2}$ - $5d_{5/2}$ ,  $5d_j$ - $6s$  matrix elements are evaluated and used to calculate lifetimes of the metastable  $5d_{5/2}$  and  $6s$  levels. The  $E1$ ,  $E2$ , and  $E3$  static polarizabilities are determined for the  $6s$  level. Scalar and tensor polarizabilities of a large number of low-lying levels are evaluated. The uncertainties of the final recommended values are estimated for all properties.

The main motivation for this work is to provide recommended values critically evaluated for their accuracy for a

number of atomic properties via a systematic high-precision study. These values may be used for astrophysics applications noted above, theoretical modeling, and planning and analysis of various experiments that may utilize interesting level structure of La III, which has metastable  $5d_{5/2}$  and  $6s$  levels.

This work was also motivated by the urgent need to study the accuracy of the theoretical description of lanthanide ions, owing to recent proposals to develop ultra-accurate atomic clocks with highly charged lanthanide ions [15,16]. Moreover, the transitions in highly charged lanthanide ions involving the  $4f$  states are particularly sensitive for the variation of the fine-structure constant  $\alpha$  [15,16]. Therefore,

accurate representation of the  $4f$  state properties is particularly important and the present work provides a benchmark test of the theoretical accuracy for these states. We also carried out a study of various contributions to the energies and transition properties of different states of La III relevant to the evaluation of accuracy of the highly charged lanthanide ion properties.

**II. CORRELATION ENERGIES OF LA III ION**

Various contributions to the energies of La III are listed in Table I in  $\text{cm}^{-1}$ . Zeroth-, second-, and third-order Coulomb correlation energies  $E^{(n)}$ ; all-order single-double (-triple)

TABLE I. Contributions to the energy levels of La III in  $\text{cm}^{-1}$ . Zeroth-, second-, and third-order Coulomb correlation energies  $E^{(n)}$ ; all-order single-double (-triple) Coulomb energies  $E^{\text{SD}}$ ;  $E^{\text{SDpT}}$ ; and the contribution of third order not included in the SD calculation,  $E^{\text{extra}}$ , are listed.  $E^{(l>6)}$  are the contributions of the higher partial waves.  $B^{(1)}$  and  $B^{(2)}$  are first-order Breit and second-order Coulomb-Breit corrections. The relative contribution of the correlation correction in % determined as the ratio of the  $E_{\text{corr}} = E^{\text{SDpT}} + E^{(l>6)}$  to the total SDpT energies is listed in the last column.

$nlj$	$E^{(0)}$	$E^{(2)}$	$E^{(3)}$	$E^{\text{SD}}$	$E^{\text{extra}}$	$E^{\text{SDpT}}$	$E^{(l>6)}$	$B^{(1)}$	$B^{(2)}$	$E_{\text{corr}} (\%)$
$5d_{3/2}$	-144 974	-11 806	3491	-10 067	1527	-8726	-319	197	-412	5.9%
$5d_{5/2}$	-143 712	-11 276	3260	-9664	1425	-8395	-309	148	-398	5.7%
$4f_{5/2}$	-114 362	-41 224	14 335	-34 044	6286	-28 877	-1210	406	-1891	21%
$4f_{7/2}$	-113 259	-40 426	13 997	-33 541	6142	-28 450	-1197	276	-1848	21%
$6s_{1/2}$	-134 360	-8556	3105	-7416	1317	-6297	-76	116	-152	4.5%
$6p_{1/2}$	-108 013	-5540	1780	-5091	791	-4375	-46	105	-86	3.9%
$6p_{3/2}$	-105 315	-5030	1612	-4627	716	-3980	-43	75	-83	3.7%
$7s_{1/2}$	-70 190	-2764	1019	-2324	430	-1985	-25	42	-53	2.8%
$6d_{3/2}$	-69 863	-2726	743	-2504	359	-2181	-52	42	-75	3.1%
$6d_{5/2}$	-69 464	-2670	723	-2459	349	-2143	-51	32	-74	3.1%
$5f_{5/2}$	-59 177	-3745	1164	-3077	547	-2642	-75	29	-126	4.4%
$5f_{7/2}$	-59 087	-3783	1179	-3074	553	-2643	-78	21	-130	4.4%
$7p_{1/2}$	-59 709	-2081	684	-1866	304	-1608	-18	44	-36	2.7%
$7p_{3/2}$	-58 597	-1927	633	-1731	280	-1491	-17	32	-35	2.5%
$8s_{1/2}$	-43 483	-1279	473	-1063	200	-910	-12	20	-25	2.1%
$7d_{3/2}$	-43 001	-1246	336	-1157	166	-1010	-22	19	-34	2.3%
$7d_{5/2}$	-42 809	-1227	331	-1143	162	-998	-22	15	-33	2.3%
$5g_{7/2}$	-39 542	-417	100	-409	56	-355	-5	0	0	0.9%
$5g_{9/2}$	-39 543	-417	100	-408	56	-354	-4	0	0	0.9%
$6f_{5/2}$	-38 170	-1872	575	-1640	273	-1404	-37	14	-61	3.6%
$6f_{7/2}$	-38 128	-1880	579	-1627	274	-1396	-38	10	-62	3.6%
$8p_{1/2}$	-38 206	-1037	342	-927	153	-800	-9	23	-18	2.1%
$8p_{3/2}$	-37 634	-969	320	-867	142	-751	-9	16	-18	2.0%
$9s_{1/2}$	-29 633	-704	260	-582	110	-499	-7	11	-14	1.7%
$8d_{3/2}$	-29 289	-690	185	-648	92	-566	-12	11	-18	1.9%
$8d_{5/2}$	-29 180	-682	183	-641	91	-561	-12	8	-18	1.9%
$6g_{7/2}$	-27 472	-275	67	-270	37	-234	-4	0	0	0.9%
$6g_{9/2}$	-27 473	-274	67	-269	37	-234	-4	0	0	0.9%
$7f_{5/2}$	-26 662	-1086	330	-984	158	-842	-22	8	-34	3.1%
$7f_{7/2}$	-26 639	-1088	332	-973	159	-834	-22	6	-35	3.1%
$9p_{1/2}$	-26 601	-597	197	-534	88	-459	-5	13	-11	1.7%
$9p_{3/2}$	-26 268	-560	186	-502	83	-434	-5	10	-11	1.6%
$10s_{1/2}$	-21 502	-436	158	-355	67	-305	-4	7	-9	1.4%
$9d_{3/2}$	-21 265	-425	113	-402	57	-425	-7	6	-11	2.0%
$9d_{5/2}$	-21 198	-420	112	-399	56	-420	-7	5	-11	2.0%
$8f_{5/2}$	-19 671	-688	207	-638	100	-688	-14	5	-21	3.4%
$8f_{7/2}$	-19 657	-688	208	-629	100	-688	-14	4	-22	3.4%
$7g_{7/2}$	-20 186	-186	45	-184	25	-159	-3	0	0	0.8%
$7g_{9/2}$	-20 187	-185	45	-183	25	-159	-3	0	0	0.8%
$8g_{7/2}$	-15 456	-128	32	-129	17	-128	-2	0	0	0.8%
$8g_{9/2}$	-15 456	-128	32	-128	17	-128	-2	0	0	0.8%

TABLE II. The total removal energies ( $\text{cm}^{-1}$ ) of La III calculated in third order and the all-order SD and SDpT approximations given in columns  $E_{\text{tot}}^{(3)}$ ,  $E_{\text{tot}}^{\text{SD}}$ , and  $E_{\text{tot}}^{\text{SDpT}}$ , compared with recommended NIST energies  $E_{\text{NIST}}$  [3]. The relative difference  $\delta E$  between experimental and theoretical results is given in the last three columns in percent.

$nlj$	$E_{\text{NIST}}$	$E_{\text{tot}}^{(3)}$	$E_{\text{tot}}^{\text{SD}}$	$E_{\text{tot}}^{\text{SDpT}}$	$\delta E^{(3)}$	$\delta E^{\text{SD}}$	$\delta E^{\text{SDpT}}$
$5d_{3/2}$	-154 675	-153 504	-154 048	-154 234	0.8	0.41	0.29
$5d_{5/2}$	-153 072	-151 978	-152 510	-152 667	0.7	0.37	0.26
$4f_{5/2}$	-147 480	-142 736	-144 816	-145 935	3.2	1.81	1.05
$4f_{7/2}$	-145 980	-141 261	-143 427	-144 478	3.2	1.75	1.03
$6s_{1/2}$	-141 084	-139 831	-140 556	-140 753	0.9	0.37	0.23
$6p_{1/2}$	-112 660	-111 755	-112 341	-112 416	0.8	0.28	0.22
$6p_{3/2}$	-109 564	-108 740	-109 277	-109 345	0.8	0.26	0.20
$7s_{1/2}$	-72 328	-71 944	-72 116	-72 208	0.5	0.29	0.17
$6d_{3/2}$	-72 294	-71 880	-72 093	-72 130	0.6	0.28	0.23
$6d_{5/2}$	-71 861	-71 454	-71 669	-71 701	0.6	0.27	0.22
$5f_{5/2}$	-62 220	-61 856	-61 880	-61 992	0.6	0.55	0.37
$5f_{7/2}$	-62 140	-61 801	-61 794	-61 916	0.6	0.56	0.36
$7p_{1/2}$	-61 443	-61 098	-61 282	-61 327	0.6	0.26	0.19
$7p_{3/2}$	-60 214	-59 893	-60 067	-60 108	0.5	0.24	0.18
$8s_{1/2}$	-44 465	-44 293	-44 362	-44 409	0.4	0.23	0.13
$7d_{3/2}$	-44 141	-43 926	-44 030	-44 048	0.5	0.25	0.21
$7d_{5/2}$	-43 937	-43 724	-43 830	-43 848	0.5	0.24	0.20
$5g_{7/2}$	-39 920	-39 860	-39 899	-39 902	0.2	0.05	0.05
$5g_{9/2}$	-39 920	-39 860	-39 899	-39 902	0.2	0.05	0.04
$6f_{5/2}$	-39 785	-39 513	-39 620	-39 657	0.7	0.42	0.32
$6f_{7/2}$	-39 736	-39 481	-39 571	-39 614	0.6	0.42	0.31
$8p_{1/2}$	-39 073	-38 897	-38 985	-39 011	0.5	0.22	0.16
$8p_{3/2}$	-38 449	-38 284	-38 369	-38 395	0.4	0.21	0.14
$9s_{1/2}$	-30 171	-30 079	-30 114	-30 141	0.3	0.19	0.10
$8d_{3/2}$	-29 933	-29 802	-29 863	-29 875	0.4	0.23	0.19
$8d_{5/2}$	-29 819	-29 689	-29 752	-29 763	0.4	0.22	0.19
$6g_{7/2}$	-27 723	-27 680	-27 709	-27 710	0.2	0.05	0.04
$6g_{9/2}$	-27 722	-27 680	-27 709	-27 710	0.2	0.05	0.04
$7f_{5/2}$	-27 632	-27 444	-27 535	-27 551	0.9	0.35	0.29
$7f_{7/2}$	-27 599	-27 424	-27 504	-27 524	0.6	0.35	0.27
$9p_{1/2}$	-27 126	-26 999	-27 050	-27 063	0.5	0.28	0.23
$9p_{3/2}$	-26 740	-26 643	-26 693	-26 707	0.4	0.18	0.12
$10s_{1/2}$	-21 835	-21 781	-21 796	-21 813	0.3	0.18	0.10
$9d_{3/2}$	-21 668	-21 582	-21 623	-21 703	0.4	0.21	-0.16
$9d_{5/2}$	-21 598	-21 513	-21 554	-21 632	0.4	0.20	-0.16
$8f_{5/2}$	-20 301	-20 168	-20 238	-20 389	0.7	0.31	-0.43
$8f_{7/2}$	-20 275	-20 155	-20 217	-20 377	0.6	0.29	-0.50
$7g_{7/2}$	-20 357	-20 327	-20 349	-20 349	0.2	0.04	0.04
$7g_{9/2}$	-20 356	-20 327	-20 348	-20 349	0.1	0.04	0.03
$8g_{7/2}$	-15 575	-15 552	-15 570	-15 586	0.2	0.03	-0.07
$8g_{9/2}$	-15 573	-15 552	-15 569	-15 586	0.1	0.02	-0.08

Coulomb energies  $E^{\text{SD}}$ ;  $E^{\text{SDpT}}$ ; and the contribution of third order not included in the SD calculation,  $E_{\text{extra}}^{(3)}$ , are given.  $E^{(l>6)}$  are the contributions of the higher partial waves.  $B^{(1)}$  and  $B^{(2)}$  are first-order Breit and second-order Coulomb-Breit corrections. The all-order single-double (SD) approximation includes the entire second-order energies but is missing a part of the third order calculated separately as  $E_{\text{extra}}^{(3)}$ . The triple-excitations terms added to the SD functions in the single-double partial triple (SDpT) all-order method (see Safronova *et al.* [17–19]) recover the part of the third-order energy missing in SD approximation. As a result,  $E_{\text{extra}}^{(3)}$  is automatically included in the SDpT energies.

As expected, the largest correlation contribution to the valence energy comes from the second-order term,  $E^{(2)}$ , which is relatively simple to calculate. Therefore, we calculate  $E^{(2)}$  with better numerical accuracy than  $E^{\text{SD}}$  and  $E^{\text{SDpT}}$  terms by including larger number of partial waves. The second-order energy  $E^{(2)}$  includes partial waves up to  $l_{\text{max}} = 8$  and is extrapolated to account for contributions from higher partial waves (see, for example, [20]). The all-order calculations are carried out with  $l_{\text{max}} = 6$ .

We display the difference between the final extrapolated second-order results and the values evaluated with  $l_{\text{max}} = 6$  in the column labeled  $E^{(l>6)}$  of Table I. We use this difference to evaluate the contribution of the higher partial waves with  $l > 6$

and add these values to the all-order energies. The relative contribution of the correlation correction in % determined as the ratio of the  $E_{\text{corr}} = E^{\text{SDpT}} + E^{(l>6)}$  to the total SDpT energies is listed in the last column of Table I. We find that the correlation correction is extremely large, 21%, for the  $4f$  states, indicating that all-order treatment is required to obtain good accuracy values of these energy levels. The contribution of the correlation correction to the energy of any other level in Table I does not exceed 6%.

The contribution of the correlation correction is the smallest, about 1%, for  $ng$  levels. The Breit correction to these levels is also very small. We note that we do not list QED correction; however, we include it in the total values. The QED contribution is the largest,  $15 \text{ cm}^{-1}$ , for the  $6s$  levels, as expected since it is the lowest valence  $ns$  level.

The total removal energies of Cs-like La III, obtained as

$$\begin{aligned} E_{\text{tot}}^{(3)} &= E^{(0)} + E^{(2)} + E^{(3)} + B^{(1+2)} + E^{(\text{QED})}, \\ E_{\text{tot}}^{\text{SD}} &= E^{(0)} + E^{\text{SD}} + E_{\text{extra}}^{(3)} + E^{(l>6)} + B^{(1+2)} + E^{(\text{QED})}, \\ E_{\text{tot}}^{\text{SDpT}} &= E^{(0)} + E^{\text{SDpT}} + E^{(l>6)} + B^{(1+2)} + E^{(\text{QED})}, \end{aligned}$$

where  $B^{(1+2)} = B^{(1)} + B^{(2)}$ , are listed in the corresponding columns of Table II. Recommended energies from the National Institute of Standards and Technology (NIST) database [3] are given in the column labeled  $E_{\text{NIST}}$ . Relative differences (in percent) between our third-order and all-order calculations and experimental data are given in the last three columns of Table II, respectively. For example, the SDpT relative difference is calculated as follows:

$$\delta E^{\text{SDpT}} = \frac{E_{\text{tot}}^{\text{SDpT}} - E_{\text{NIST}}}{E_{\text{NIST}}}.$$

The SDpT approximation includes the most correlation correction terms and generally gives the results in closest agreement with the experiment, in particular for the  $nf$  levels where the correlation correction is the largest. The all-order results are in excellent agreement with the experiment, differing with the experiment by 0.03–0.3% for most levels.

### III. ELECTRIC DIPOLE MATRIX ELEMENTS, OSCILLATOR STRENGTHS, TRANSITION RATES, AND LIFETIMES IN CS-LIKE LA<sup>2+</sup>

#### A. Electric dipole matrix elements

In Table III, we list our recommended values for 129  $E1$   $ns - n'p$ ,  $nd - n'p$ ,  $nd - n'f$ , and  $ng - n'f$  transitions. The absolute values in atomic units ( $a_0e$ ) are given. We note that we have calculated all 237  $E1$  matrix elements between the  $ns$ ,  $np$ ,  $nd$ ,  $nf$ , and  $ng$  states with  $n \leq 8$  but we only list the matrix elements that give significant contributions to the atomic lifetimes and polarizabilities calculated in the other sections. To evaluate the uncertainties of these values, we carried out a number of calculations using different methods of increasing accuracy: lowest-order DF, second-order relativistic many-body perturbation theory (RMBPT), third-order RMBPT, and the all-order methods. The RMBPT calculations are carried out using the method described in [21]. We compared the values obtained in different approximations to evaluate the size of the second-, third-, and higher-order correlation corrections.

The evaluation of the uncertainty of the matrix elements was described in detail in [22,23]. The uncertainty is evaluated based on four different all-order calculations that included two *ab initio* all-order calculations with and without the inclusion of the partial triple excitations and two calculations that included a semiempirical estimate of high-order correlation corrections starting from both *ab initio* runs. We have developed an algorithm that accounted for the importance of the specific dominant contributions and allowed us to use the differences of these four values for each transition to estimate uncertainty of the final results.

The column labeled “%” of Table III gives relative uncertainties of the final values  $Z^{\text{final}}$  in percent. The values of uncertainties for the 129  $E1$  transitions given in Table III are smaller than 2%. We find that the uncertainties are 0.1–0.3% for the  $ns-n'p$  transitions. Larger uncertainties (0.5–1.9%) occur for some of the  $nd-n'p$ ,  $nd-n'f$ , and  $ng-n'f$  transitions owing to the increased relative size of the correlation corrections. The values of uncertainties in Cs-like La<sup>2+</sup> are larger than the values of uncertainties in Rb-like Y<sup>2+</sup> [20] and in K-like Sc<sup>2+</sup> [23], as expected, due to the increased size of the core.

The problem with evaluation of matrix elements in La III involving the  $4f$  and  $5d$  orbitals was investigated by Migdalek and Wyrozumska [7]. Inclusion of the local valence-core electron exchange interaction in the effective potential affects the behavior of the inner and outer wells of this potential and therefore greatly facilitates the collapse of  $4f$  and  $5d$  orbitals along the sequence. In the collapse region, the properties of the  $5d$  and  $4f$  orbitals are unusually sensitive to small perturbations [7]. Safronova [24] mentioned that the all-order method did not converge for  $nf$  states in Cs-like Ba<sup>+</sup>. The form-independent third-order perturbation theory approach developed by Savukov and Johnson in [25] was used to evaluate the multipole reduced matrix elements that include the  $nf$  states.

As a result, our work provides the most accurate values of the matrix elements of the lanthanide ion involving  $nf$  states due to our accurate treatment of the correlation corrections. Our final results and their uncertainties are used to calculate the recommended values of the transition rates, oscillator strengths, and lifetimes discussed below.

#### B. Transition rates and oscillator strengths

We combine recommended NIST energies [3] and our final values of the matrix elements listed in Table III to calculate weighted transition rates  $gA_r$  and weighted oscillator strengths  $gf$ . The weighted transition rates  $gA_r$  are calculated using

$$gA_r = \frac{2.02613 \times 10^{18}}{\lambda^3} \times S \text{ s}^{-1}, \quad (1)$$

where the wavelength  $\lambda$  is in Å and the line strength  $S = D^2$  is in atomic units.

Transition rates  $gA$  ( $\text{s}^{-1}$ ) for the 94 allowed electric dipole transitions between  $ns$ ,  $np$ ,  $nd$ ,  $nf$ , and  $ng$  states with  $n \leq 8$  are listed Table IV. Vacuum wavelengths obtained from NIST energies are also listed for reference. The transitions are ordered by the value of the wavelength. The relative uncertainties of the transition rates are twice the corresponding matrix

TABLE III. Recommended values of the reduced electric dipole matrix elements in Cs-like La III in atomic units. Final recommended values and their uncertainties are given in the  $Z^{\text{final}}$  column. The column (%) gives relative uncertainties of the final values in %. The lowest-order DF values are displayed in the  $Z^{\text{DF}}$  column for reference. Absolute values are given.

Transition	DHF	Final	Unc.	Transition	DHF	Final	Unc.	Transition	DHF	Final	Unc.
6s-6p <sub>1/2</sub>	3.250	2.780(8)	0.3%	6d <sub>3/2</sub> -8p <sub>3/2</sub>	0.289	0.275(2)	0.9%	6d <sub>5/2</sub> -5f <sub>7/2</sub>	11.37	10.31(9)	0.9%
6s-6p <sub>3/2</sub>	4.577	3.93(3)	0.7%	6d <sub>5/2</sub> -8p <sub>3/2</sub>	0.834	0.79(1)	1.3%	6d <sub>3/2</sub> -7f <sub>5/2</sub>	1.559	1.75(3)	1.6%
6s-8p <sub>1/2</sub>	0.053	0.146(2)	1.6%	6d <sub>3/2</sub> -9p <sub>3/2</sub>	0.140	0.129(1)	1.1%	6d <sub>5/2</sub> -7f <sub>5/2</sub>	0.431	0.481(7)	1.5%
7s-6p <sub>1/2</sub>	1.873	1.83(1)	0.6%	6d <sub>5/2</sub> -9p <sub>3/2</sub>	0.404	0.370(5)	1.3%	6d <sub>5/2</sub> -7f <sub>7/2</sub>	1.913	2.14(3)	1.5%
7s-6p <sub>3/2</sub>	2.954	2.90(1)	0.4%	7d <sub>3/2</sub> -6p <sub>1/2</sub>	1.065	0.88(1)	1.6%	7d <sub>3/2</sub> -6f <sub>5/2</sub>	16.50	15.70(8)	0.5%
7s-7p <sub>1/2</sub>	5.861	5.56(2)	0.3%	7d <sub>3/2</sub> -6p <sub>3/2</sub>	0.451	0.363(7)	1.8%	7d <sub>5/2</sub> -6f <sub>5/2</sub>	4.424	4.20(2)	0.5%
7s-7p <sub>3/2</sub>	8.185	7.77(3)	0.4%	7d <sub>5/2</sub> -6p <sub>3/2</sub>	1.387	1.129(9)	0.8%	7d <sub>5/2</sub> -6f <sub>7/2</sub>	19.79	18.82(9)	0.5%
8s-6p <sub>1/2</sub>	0.545	0.548(2)	0.4%	7d <sub>3/2</sub> -7p <sub>1/2</sub>	7.410	7.21(6)	0.8%	8d <sub>3/2</sub> -5f <sub>5/2</sub>	0.809	0.75(1)	1.9%
8s-6p <sub>3/2</sub>	0.811	0.808(3)	0.4%	7d <sub>3/2</sub> -7p <sub>3/2</sub>	3.524	3.42(2)	0.6%	8d <sub>5/2</sub> -5f <sub>5/2</sub>	0.212	0.197(4)	1.9%
8s-7p <sub>1/2</sub>	3.560	3.473(8)	0.2%	7d <sub>5/2</sub> -7p <sub>3/2</sub>	10.44	10.13(7)	0.7%	8d <sub>5/2</sub> -5f <sub>7/2</sub>	0.957	0.89(2)	2.0%
8s-7p <sub>3/2</sub>	5.547	5.430(8)	0.2%	7d <sub>3/2</sub> -8p <sub>1/2</sub>	10.62	10.25(5)	0.5%	8d <sub>3/2</sub> -7f <sub>5/2</sub>	24.87	24.09(8)	0.4%
8s-8p <sub>1/2</sub>	9.179	8.93(2)	0.2%	7d <sub>3/2</sub> -8p <sub>3/2</sub>	4.589	4.42(2)	0.5%	8d <sub>5/2</sub> -7f <sub>5/2</sub>	6.669	6.45(2)	0.4%
8s-8p <sub>3/2</sub>	12.77	12.42(3)	0.2%	7d <sub>5/2</sub> -8p <sub>3/2</sub>	13.98	13.47(7)	0.5%	8d <sub>5/2</sub> -7f <sub>7/2</sub>	29.83	28.9(1)	0.4%
9s-6p <sub>1/2</sub>	0.299	0.303(1)	0.5%	7d <sub>3/2</sub> -9p <sub>1/2</sub>	0.691	0.67(1)	1.5%	9d <sub>3/2</sub> -6f <sub>5/2</sub>	1.604	1.45(3)	1.8%
9s-6p <sub>3/2</sub>	0.440	0.439(2)	0.5%	7d <sub>3/2</sub> -9p <sub>3/2</sub>	0.402	0.403(4)	1.0%	9d <sub>5/2</sub> -6f <sub>5/2</sub>	0.422	0.381(7)	1.9%
9s-7p <sub>1/2</sub>	0.953	0.948(2)	0.3%	7d <sub>5/2</sub> -9p <sub>3/2</sub>	1.137	1.14(1)	1.1%	9d <sub>5/2</sub> -6f <sub>7/2</sub>	1.897	1.72(3)	1.9%
9s-7p <sub>3/2</sub>	1.392	1.381(4)	0.3%	8d <sub>3/2</sub> -7p <sub>1/2</sub>	1.778	1.66(2)	1.3%	9d <sub>3/2</sub> -8f <sub>5/2</sub>	34.64	33.9(1)	0.4%
9s-8p <sub>1/2</sub>	5.686	5.54(1)	0.2%	8d <sub>3/2</sub> -7p <sub>3/2</sub>	0.764	0.70(1)	1.5%	9d <sub>5/2</sub> -8f <sub>5/2</sub>	9.294	9.09(4)	0.4%
9s-8p <sub>3/2</sub>	8.807	8.61(2)	0.2%	8d <sub>5/2</sub> -7p <sub>3/2</sub>	2.334	2.16(3)	1.4%	9d <sub>5/2</sub> -8f <sub>7/2</sub>	41.56	40.6(2)	0.4%
9s-9p <sub>1/2</sub>	13.21	12.995(8)	0.06%	8d <sub>3/2</sub> -8p <sub>1/2</sub>	10.78	10.64(7)	0.6%				
9s-9p <sub>3/2</sub>	18.33	17.995(9)	0.05%	8d <sub>3/2</sub> -8p <sub>3/2</sub>	5.146	5.09(4)	0.7%	5g <sub>7/2</sub> -5f <sub>5/2</sub>	11.96	10.7(1)	1.3%
10s-6p <sub>1/2</sub>	0.201	0.204(1)	0.5%	8d <sub>5/2</sub> -8p <sub>3/2</sub>	15.22	15.1(1)	0.8%	5g <sub>7/2</sub> -5f <sub>7/2</sub>	2.308	2.06(3)	1.3%
10s-6p <sub>3/2</sub>	0.294	0.294(1)	0.5%	8d <sub>3/2</sub> -9p <sub>1/2</sub>	16.18	15.74(4)	0.3%	5g <sub>9/2</sub> -5f <sub>7/2</sub>	13.65	12.2(2)	1.3%
10s-7p <sub>1/2</sub>	0.506	0.507(2)	0.4%	8d <sub>3/2</sub> -9p <sub>3/2</sub>	6.998	6.78(4)	0.5%	5g <sub>7/2</sub> -6f <sub>5/2</sub>	12.99	13.48(9)	0.7%
10s-7p <sub>3/2</sub>	0.728	0.727(2)	0.3%	8d <sub>5/2</sub> -9p <sub>3/2</sub>	21.29	20.6(1)	0.5%	5g <sub>7/2</sub> -6f <sub>7/2</sub>	2.494	2.59(2)	0.7%
10s-8p <sub>1/2</sub>	1.458	1.440(4)	0.3%	9d <sub>3/2</sub> -8p <sub>1/2</sub>	2.623	2.52(3)	1.3%	5g <sub>9/2</sub> -6f <sub>7/2</sub>	14.75	15.3(1)	0.7%
10s-8p <sub>3/2</sub>	2.107	2.082(6)	0.3%	9d <sub>3/2</sub> -8p <sub>3/2</sub>	1.137	1.08(2)	1.9%	6g <sub>7/2</sub> -5f <sub>5/2</sub>	2.797	2.90(5)	1.7%
10s-9p <sub>1/2</sub>	8.261	8.00(7)	0.8%	9d <sub>5/2</sub> -8p <sub>3/2</sub>	3.461	3.31(6)	1.7%	6g <sub>7/2</sub> -5f <sub>7/2</sub>	0.534	0.56(1)	1.9%
10s-9p <sub>3/2</sub>	12.75	12.49(1)	0.1%	9d <sub>3/2</sub> -9p <sub>1/2</sub>	14.73	14.6(2)	1.7%	6g <sub>9/2</sub> -5f <sub>7/2</sub>	3.160	3.29(6)	1.9%
								6g <sub>7/2</sub> -7f <sub>5/2</sub>	23.53	24.3(1)	0.5%
5d <sub>3/2</sub> -6p <sub>1/2</sub>	2.526	2.14(2)	0.8%	5d <sub>3/2</sub> -4f <sub>5/2</sub>	2.364	1.30(4)	2.8%	6g <sub>7/2</sub> -7f <sub>7/2</sub>	4.520	4.66(2)	0.5%
5d <sub>3/2</sub> -6p <sub>3/2</sub>	1.083	0.922(8)	0.8%	5d <sub>5/2</sub> -4f <sub>5/2</sub>	0.631	0.35(1)	2.8%	6g <sub>9/2</sub> -7f <sub>7/2</sub>	26.74	27.6(1)	0.5%
5d <sub>5/2</sub> -6p <sub>3/2</sub>	3.334	2.85(2)	0.8%	5d <sub>5/2</sub> -4f <sub>7/2</sub>	2.867	1.59(5)	2.9%	7g <sub>7/2</sub> -6f <sub>5/2</sub>	4.668	4.66(2)	0.5%
5d <sub>3/2</sub> -7p <sub>1/2</sub>	0.466	0.319(6)	1.9%	5d <sub>3/2</sub> -5f <sub>5/2</sub>	2.436	2.31(2)	1.1%	7g <sub>7/2</sub> -6f <sub>7/2</sub>	0.896	0.897(5)	0.6%
5d <sub>3/2</sub> -7p <sub>3/2</sub>	0.220	0.161(2)	1.5%	5d <sub>5/2</sub> -5f <sub>5/2</sub>	0.671	0.639(6)	1.0%	7g <sub>9/2</sub> -6f <sub>7/2</sub>	5.302	5.31(3)	0.6%
5d <sub>5/2</sub> -7p <sub>3/2</sub>	0.658	0.482(8)	1.6%	5d <sub>5/2</sub> -5f <sub>7/2</sub>	2.969	2.84(3)	1.2%	7g <sub>7/2</sub> -8f <sub>5/2</sub>	35.54	36.5(3)	0.9%
5d <sub>5/2</sub> -8p <sub>3/2</sub>	0.354	0.231(5)	2.0%	5d <sub>3/2</sub> -6f <sub>5/2</sub>	1.369	1.12(1)	1.1%	7g <sub>7/2</sub> -8f <sub>7/2</sub>	6.829	7.02(7)	1.0%
6d <sub>3/2</sub> -6p <sub>1/2</sub>	4.592	4.21(2)	0.5%	5d <sub>5/2</sub> -6f <sub>5/2</sub>	0.373	0.307(3)	1.0%	7g <sub>9/2</sub> -8f <sub>7/2</sub>	40.39	41.5(4)	1.0%
6d <sub>3/2</sub> -6p <sub>3/2</sub>	2.171	1.998(9)	0.5%	5d <sub>5/2</sub> -6f <sub>7/2</sub>	1.659	1.38(1)	1.0%	8g <sub>7/2</sub> -6f <sub>5/2</sub>	2.335	2.47(3)	1.1%
6d <sub>5/2</sub> -6p <sub>3/2</sub>	6.452	5.94(3)	0.5%	5d <sub>3/2</sub> -7f <sub>5/2</sub>	0.920	0.68(1)	1.6%	8g <sub>7/2</sub> -6f <sub>7/2</sub>	0.447	0.474(5)	1.1%
6d <sub>3/2</sub> -7p <sub>1/2</sub>	6.091	5.78(3)	0.5%	5d <sub>5/2</sub> -7f <sub>7/2</sub>	1.113	0.84(1)	1.5%	8g <sub>9/2</sub> -6f <sub>7/2</sub>	2.644	2.81(3)	1.2%
6d <sub>3/2</sub> -7p <sub>3/2</sub>	2.624	2.49(1)	0.5%	5d <sub>5/2</sub> -8f <sub>5/2</sub>	0.184	0.124(2)	1.9%	8g <sub>7/2</sub> -7f <sub>5/2</sub>	6.478	6.29(4)	0.6%
6d <sub>5/2</sub> -7p <sub>3/2</sub>	8.014	7.61(4)	0.5%	6d <sub>3/2</sub> -5f <sub>5/2</sub>	9.485	8.60(7)	0.8%	8g <sub>7/2</sub> -7f <sub>7/2</sub>	1.246	1.212(7)	0.6%
6d <sub>3/2</sub> -8p <sub>1/2</sub>	0.540	0.501(8)	1.6%	6d <sub>5/2</sub> -5f <sub>5/2</sub>	2.539	2.30(2)	0.9%	8g <sub>9/2</sub> -7f <sub>7/2</sub>	7.372	7.17(4)	0.6%

element uncertainties. The uncertainties in percent are listed in the column labeled “Unc.” The largest uncertainties (about 2%) are for the  $5d-nf$  transitions, while the smallest ones (about 0.3%) are for the  $ns-n'p$  transitions as we discussed in the previous section. Larger uncertainties generally result from larger relative size of the correlation corrections.

The theoretical transition probabilities in  $\text{La}^{2+}$  were obtained using a multiconfiguration relativistic Hartree-Fock method including core polarization in [9]. We did not repeat  $gA_r$ [9] values from Table I of [9]; however, we ordered our  $gA_r^{\text{final}}$  values with the level of the disagreement with the results

from [9]. Since our results include the correlation correction in a much more complete way, we expect much larger differences with [9] for the transitions where the correlation correction contribution is large.

In the left column of Table IV, we displayed  $gA_r^{\text{final}}$  values for 47 transitions. The correlation corrections contribute less than 10% for the first 25 transitions. As a result, the difference between our  $gA_r^{\text{final}}$  values and the  $gA_r$  values from [9] is also less than 10%.

We find substantially larger disagreement (11–40%) between  $gA_r^{\text{final}}$  and  $gA_r$ [9] for the transition presented in the

TABLE IV. Weighted oscillator strengths ( $gf$ ) and transition rates  $gA_r$  ( $s^{-1}$ ) in Cs-like La III calculated using our recommended values of reduced electric dipole matrix elements. The relative uncertainties of the final values are listed in column "Unc." in %. The vacuum wavelengths  $\lambda$  in Å from the NIST compilation [3] are listed for reference. Numbers in brackets represent powers of 10.

Transition						Transition					
Lower	Upper	$\lambda$ (Å)	$gf$	$gA_r$ ( $s^{-1}$ )	Unc.	Lower	Upper	$\lambda$ (Å)	$gf$	$gA_r$ ( $s^{-1}$ )	Unc.
6p <sub>3/2</sub>	10s <sub>1/2</sub>	1139.87	0.023	1.18 [8]	1.0%	6d <sub>5/2</sub>	9p <sub>3/2</sub>	2216.27	0.019	2.55 [7]	2.7%
6p <sub>3/2</sub>	8s <sub>1/2</sub>	1536.13	0.129	3.64 [8]	0.8%	6d <sub>3/2</sub>	7f <sub>5/2</sub>	2239.05	0.417	5.55 [8]	3.2%
7p <sub>1/2</sub>	10s <sub>1/2</sub>	2524.74	0.031	3.24 [7]	0.8%	6d <sub>5/2</sub>	7f <sub>7/2</sub>	2259.31	0.613	8.02 [8]	2.9%
7p <sub>3/2</sub>	10s <sub>1/2</sub>	2605.59	0.062	6.05 [7]	0.6%	6d <sub>5/2</sub>	7f <sub>5/2</sub>	2261.00	0.031	4.05 [7]	2.9%
6d <sub>5/2</sub>	8p <sub>3/2</sub>	2992.97	0.064	4.75 [7]	2.7%	5f <sub>5/2</sub>	7g <sub>7/2</sub>	2388.72	0.246	2.88 [8]	4.9%
7p <sub>1/2</sub>	9s <sub>1/2</sub>	3197.78	0.085	5.56 [7]	0.5%	5f <sub>5/2</sub>	6g <sub>7/2</sub>	2898.72	0.883	7.01 [8]	3.5%
7p <sub>3/2</sub>	9s <sub>1/2</sub>	3328.60	0.174	1.05 [8]	0.5%	5f <sub>7/2</sub>	6g <sub>9/2</sub>	2905.42	1.134	8.96 [8]	3.8%
6f <sub>5/2</sub>	7g <sub>7/2</sub>	5147.15	1.283	3.23 [8]	1.1%	5f <sub>7/2</sub>	6g <sub>7/2</sub>	2905.48	0.032	2.56 [7]	3.7%
6f <sub>7/2</sub>	7g <sub>9/2</sub>	5159.83	1.658	4.15 [8]	1.2%	5f <sub>5/2</sub>	8d <sub>5/2</sub>	3086.27	0.004	2.68 [6]	3.8%
6f <sub>7/2</sub>	7g <sub>7/2</sub>	5160.19	0.047	1.19 [7]	1.1%	5f <sub>7/2</sub>	8d <sub>5/2</sub>	3093.93	0.078	5.40 [7]	3.9%
8p <sub>1/2</sub>	9d <sub>3/2</sub>	5745.68	0.336	6.79 [7]	2.7%	5f <sub>5/2</sub>	8d <sub>3/2</sub>	3097.15	0.056	3.87 [7]	3.7%
7p <sub>1/2</sub>	7d <sub>3/2</sub>	5779.74	2.730	5.45 [8]	1.6%	7p <sub>3/2</sub>	8d <sub>3/2</sub>	3302.42	0.045	2.78 [7]	3.0%
8p <sub>1/2</sub>	10s <sub>1/2</sub>	5801.09	0.109	2.15 [7]	0.5%	6f <sub>5/2</sub>	8g <sub>7/2</sub>	4130.41	0.449	1.75 [8]	2.3%
7d <sub>5/2</sub>	9p <sub>3/2</sub>	5815.06	0.068	1.34 [7]	2.3%	6f <sub>7/2</sub>	8g <sub>9/2</sub>	4138.59	0.577	2.25 [8]	2.3%
8p <sub>3/2</sub>	10s <sub>1/2</sub>	6018.84	0.219	4.03 [7]	0.6%	6f <sub>7/2</sub>	8g <sub>7/2</sub>	4138.80	0.016	6.42 [6]	2.3%
7p <sub>3/2</sub>	7d <sub>5/2</sub>	6143.69	5.073	8.96 [8]	1.3%	6f <sub>5/2</sub>	9d <sub>5/2</sub>	5498.40	0.008	1.77 [6]	3.9%
7p <sub>3/2</sub>	7d <sub>3/2</sub>	6221.71	0.570	9.82 [7]	1.3%	6f <sub>7/2</sub>	9d <sub>5/2</sub>	5513.29	0.162	3.56 [7]	3.8%
7p <sub>3/2</sub>	8s <sub>1/2</sub>	6349.96	1.410	2.33 [8]	0.3%	6f <sub>5/2</sub>	9d <sub>3/2</sub>	5519.72	0.116	2.55 [7]	3.6%
7s <sub>1/2</sub>	7p <sub>3/2</sub>	8254.80	2.220	2.17 [8]	0.7%	7p <sub>1/2</sub>	8s <sub>1/2</sub>	5890.26	0.622	1.20 [8]	0.5%
6d <sub>3/2</sub>	7p <sub>3/2</sub>	8277.68	0.228	2.22 [7]	0.9%						
7f <sub>5/2</sub>	8g <sub>7/2</sub>	8293.32	1.447	1.40 [8]	1.2%	5d <sub>3/2</sub>	8f <sub>5/2</sub>	744.19	0.086	1.03 [9]	5.0%
7f <sub>7/2</sub>	8g <sub>9/2</sub>	8315.25	1.877	1.81 [8]	1.1%	5d <sub>5/2</sub>	8f <sub>7/2</sub>	753.03	0.131	1.54 [9]	4.8%
7f <sub>7/2</sub>	8g <sub>7/2</sub>	8316.09	0.054	5.17 [6]	1.1%	5d <sub>5/2</sub>	8f <sub>5/2</sub>	753.18	0.006	7.32 [7]	3.7%
6d <sub>5/2</sub>	7p <sub>3/2</sub>	8585.78	2.050	1.85 [8]	1.0%	5d <sub>3/2</sub>	9p <sub>3/2</sub>	781.65	0.001	9.37 [6]	5.5%
7s <sub>1/2</sub>	7p <sub>1/2</sub>	9186.86	1.022	8.08 [7]	0.7%	5d <sub>3/2</sub>	7f <sub>5/2</sub>	787.14	0.177	1.90 [9]	3.2%
						5d <sub>5/2</sub>	9p <sub>3/2</sub>	791.57	0.008	8.08 [7]	6.0%
5d <sub>5/2</sub>	7f <sub>7/2</sub>	796.99	0.266	2.79 [9]	2.9%	5d <sub>5/2</sub>	7f <sub>5/2</sub>	797.20	0.013	1.36 [8]	4.3%
5d <sub>3/2</sub>	6f <sub>5/2</sub>	870.40	0.439	3.87 [9]	2.1%	5d <sub>3/2</sub>	8p <sub>3/2</sub>	860.39	0.002	1.89 [7]	4.4%
5d <sub>5/2</sub>	6f <sub>7/2</sub>	882.33	0.654	5.60 [9]	1.9%	5d <sub>5/2</sub>	8p <sub>3/2</sub>	872.43	0.018	1.62 [8]	3.9%
5d <sub>5/2</sub>	6f <sub>5/2</sub>	882.72	0.032	2.78 [8]	2.0%	5d <sub>3/2</sub>	7p <sub>3/2</sub>	1058.63	0.007	4.43 [7]	3.0%
5d <sub>3/2</sub>	5f <sub>5/2</sub>	1081.61	1.501	8.56 [9]	2.1%	5d <sub>3/2</sub>	7p <sub>1/2</sub>	1072.59	0.029	1.67 [8]	3.8%
6p <sub>3/2</sub>	7d <sub>5/2</sub>	1523.75	0.254	7.30 [8]	1.6%	5d <sub>5/2</sub>	7p <sub>3/2</sub>	1076.91	0.066	3.77 [8]	3.2%
6d <sub>3/2</sub>	9p <sub>3/2</sub>	2195.18	0.002	3.21 [6]	2.1%	6p <sub>3/2</sub>	7d <sub>3/2</sub>	1528.51	0.026	7.49 [7]	3.7%
5d <sub>5/2</sub>	6p <sub>3/2</sub>	2298.44	1.076	1.36 [9]	1.7%	6d <sub>3/2</sub>	9p <sub>1/2</sub>	2213.95	0.007	9.81 [6]	4.5%
5d <sub>3/2</sub>	6p <sub>1/2</sub>	2380.10	0.585	6.89 [8]	1.6%	5d <sub>3/2</sub>	6p <sub>3/2</sub>	2216.76	0.117	1.58 [8]	1.6%
6p <sub>3/2</sub>	6d <sub>5/2</sub>	2652.29	4.045	3.84 [9]	0.9%	6p <sub>1/2</sub>	7s <sub>1/2</sub>	2479.41	0.412	4.47 [8]	1.1%
6p <sub>3/2</sub>	6d <sub>3/2</sub>	2683.14	0.452	4.19 [8]	0.9%	6d <sub>3/2</sub>	8p <sub>1/2</sub>	3010.10	0.025	1.86 [7]	3.1%
6p <sub>3/2</sub>	7s <sub>1/2</sub>	2685.55	0.951	8.80 [8]	0.7%	6d <sub>3/2</sub>	6f <sub>5/2</sub>	3076.07	1.021	7.20 [8]	5.5%
6d <sub>3/2</sub>	8p <sub>3/2</sub>	2954.63	0.008	5.95 [6]	1.8%	6d <sub>5/2</sub>	6f <sub>7/2</sub>	3112.88	1.535	1.06 [9]	5.2%
6s <sub>1/2</sub>	6p <sub>3/2</sub>	3172.61	1.478	9.79 [8]	1.4%	5f <sub>5/2</sub>	7d <sub>5/2</sub>	5469.33	0.029	6.56 [6]	5.4%
7p <sub>1/2</sub>	8d <sub>3/2</sub>	3173.61	0.263	1.74 [8]	2.5%	5f <sub>7/2</sub>	7d <sub>5/2</sub>	5493.42	0.598	1.32 [8]	5.6%
7p <sub>3/2</sub>	8d <sub>5/2</sub>	3290.05	0.429	2.64 [8]	2.9%	5f <sub>5/2</sub>	7d <sub>3/2</sub>	5531.08	0.435	9.49 [7]	5.3%
6s <sub>1/2</sub>	6p <sub>1/2</sub>	3518.17	0.667	3.60 [8]	0.6%	7d <sub>3/2</sub>	9p <sub>1/2</sub>	5877.26	0.023	4.52 [6]	3.0%
5f <sub>5/2</sub>	5g <sub>7/2</sub>	4484.23	7.695	2.55 [9]	2.6%	7d <sub>3/2</sub>	7f <sub>5/2</sub>	6057.53	0.814	1.48 [8]	6.8%
5f <sub>7/2</sub>	5g <sub>9/2</sub>	4500.33	9.998	3.29 [9]	2.7%	7d <sub>5/2</sub>	7f <sub>7/2</sub>	6120.97	1.238	2.20 [8]	6.3%
5f <sub>7/2</sub>	5g <sub>7/2</sub>	4500.42	0.286	9.41 [7]	2.7%	6f <sub>5/2</sub>	6g <sub>7/2</sub>	8290.04	7.209	7.00 [8]	4.1%
6d <sub>3/2</sub>	7p <sub>1/2</sub>	9215.21	1.103	8.66 [7]	0.9%	6f <sub>7/2</sub>	6g <sub>9/2</sub>	8323.44	9.409	9.06 [8]	4.1%
6d <sub>3/2</sub>	5f <sub>5/2</sub>	9926.76	2.261	1.53 [8]	1.7%	6f <sub>7/2</sub>	6g <sub>7/2</sub>	8323.92	0.269	2.59 [7]	4.1%

right column of Table IV. The differences are attributed to omitted higher-order correlation corrections in [9]. The  $gA_r$  values from [9] are in good agreement with our  $gA_r^{\text{DF}}$  values, as expected. To verify this, we used the reduced matrix elements obtained in the DF approach given in Table III to calculate

$gA_r^{\text{DF}}$  values using DF values for matrix elements and NIST energies. We find small (less than 10%) differences for the 19 transitions displayed in the right column of Table IV between the  $gA_r$  [9] and  $gA_r^{\text{DF}}$  values. The  $gA_r$  [9] values are in disagreement with  $gA_r^{\text{final}}$  and  $gA_r^{\text{DF}}$  values for the 28

TABLE V. Lifetimes ( $\tau^{\text{final}}$  in ns) of La III levels. Uncertainties are given in parentheses. Recommended NIST energies [3] are given in  $\text{cm}^{-1}$ . The values of lifetimes evaluated in the DF approximation are given in column  $\tau^{\text{DF}}$  to illustrate the importance of the correlation corrections. Theoretical values from [13] and experimental measurements from [10] are listed in the last two columns.

Level	Energy [3]	$\tau^{\text{DF}}$	$\tau^{\text{final}}$	$\tau^{\text{theory}}$ [13]	$\tau^{\text{expt}}$ [10]
4f <sub>5/2</sub>	7195.14	1376	4560(240)	2284	
4f <sub>7/2</sub>	8695.41	1348	4370(260)	2301	
6p <sub>1/2</sub>	42 015.04	1.377	1.908(20)	1.537	1.95(20)
6p <sub>3/2</sub>	45 110.94	1.176	1.601(17)	1.271	1.56(20)
7s <sub>1/2</sub>	82 347.28	1.451	1.508(09)	1.546	
6d <sub>3/2</sub>	82 380.76	1.153	1.409(14)	1.199	
6d <sub>5/2</sub>	82 814.27	1.260	1.531(16)	1.419	
5f <sub>5/2</sub>	92 454.54	0.579	0.641(12)	0.590	
5f <sub>7/2</sub>	92 534.73	0.585	0.639(15)	0.619	
7p <sub>1/2</sub>	93 232.39	3.678	5.408(98)	3.365	
7p <sub>3/2</sub>	94 461.44	3.154	4.666(68)	3.262	
8s <sub>1/2</sub>	110 209.57	2.154	2.196(08)	2.212	
7d <sub>3/2</sub>	110 534.20	2.364	2.956(46)	2.486	
7d <sub>5/2</sub>	110 738.31	2.621	3.289(39)	2.793	
5g <sub>7/2</sub>	114 754.90	1.469	2.554(76)	2.262	
5g <sub>9/2</sub>	114 755.34	1.453	2.551(81)	2.295	
6f <sub>5/2</sub>	114 889.80	0.891	1.208(22)	0.935	
6f <sub>7/2</sub>	114 938.90	0.903	1.192(22)	0.972	
8p <sub>1/2</sub>	115 602.26	7.165	10.82(28)	6.699	
8p <sub>3/2</sub>	116 225.92	6.295	9.83(16)	6.398	
9s <sub>1/2</sub>	124 504.10	3.357	3.391(12)	3.403	
8d <sub>3/2</sub>	124 742.24	4.175	5.325(89)	4.436	
8d <sub>5/2</sub>	124 856.08	4.676	5.96(12)	4.851	
6g <sub>7/2</sub>	126 952.47	2.408	4.24(13)	3.841	
6g <sub>9/2</sub>	126 953.16	2.384	4.22(15)	3.901	
7f <sub>5/2</sub>	127 042.58	1.379	2.133(49)	1.448	
7f <sub>7/2</sub>	127 075.60	1.391	2.085(47)	1.498	
9p <sub>1/2</sub>	127 548.93	12.28	18.90(85)	11.35	
9p <sub>3/2</sub>	127 935.04	10.93	17.80(41)	11.04	
10s <sub>1/2</sub>	132 840.41	5.068	5.091(19)	5.105	
9d <sub>3/2</sub>	133 006.65	6.700	8.65(27)	7.159	
9d <sub>5/2</sub>	133 076.90	7.545	9.76(30)	7.723	
7g <sub>7/2</sub>	134 318.02	3.725	6.60(21)	6.061	
7g <sub>9/2</sub>	134 319.39	3.685	6.56(23)	6.158	
8f <sub>5/2</sub>	134 373.83	2.057	3.50(13)	2.159	
8f <sub>7/2</sub>	134 399.63	2.049	3.29(12)	2.228	
8g <sub>7/2</sub>	139 100.48	5.456	9.75(34)	9.007	
8g <sub>9/2</sub>	139 101.70	5.400	9.67(37)	9.156	

transitions displayed in the bottom of the right column of Table IV. The correlation corrections are particularly large for these cases, leading to large uncertainties shown in column ‘‘Unc.’’ of Table IV. [9].

### C. Lifetimes of La III levels

We calculated lifetimes of the *ns* ( $n = 7-10$ ), *np* ( $n = 6-9$ ), *nd* ( $n = 6-9$ ), *nf* ( $n = 4-8$ ), and *ng* ( $n = 5-8$ ) states in La III using our final values of the transition rates listed in Table IV. The lifetimes of the metastable *5d<sub>5/2</sub>* and *6s* states are discussed in the next section. The recommended NIST energies [3] are given in column ‘‘Energy’’ for reference. We

also included the lowest-order DF lifetimes  $\tau^{\text{DF}}$  to illustrate the size of the correlation effects. Our final results are given in columns  $\tau^{\text{final}}$  of Table V. The uncertainties in the lifetime values are obtained from the uncertainties in the transition rates listed in Table IV.

The present values are compared with theoretical results obtained by Karaçoban and Özdemir [13] using the HFR method developed by Cowan [8] (see column  $\tau^{\text{theory}}$  in Table V). We find good agreement (3–11%) between  $\tau^{\text{final}}$  and lifetimes from [13] for the *ns* and *ng* ( $n = 5-9$ ) states. Lifetimes of *np*, *nd*, and *nf* levels presented by Karaçoban and Özdemir [13] disagree substantially (10–40%) with our results; however, they are in very good agreement (1–10%) with the  $\tau^{\text{DF}}$ . This indicates that the disagreement is due to omission of the important correlation corrections in [13] for these states. The largest contribution of the correlation correction is for the lifetimes of the *4f* levels: the values of the  $\tau^{\text{final}}$  and  $\tau^{\text{DF}}$  differ by a factor of 3.3.

There are no experimental measurements of the La III lifetimes with the exceptions of the *6p* levels presented by Li and Zhankui [10]. Our  $\tau^{\text{final}}$  values are in agreement with these measurements within the uncertainties; however, our values are ten times more accurate than the experimental measurements.

### IV. ELECTRIC QUADRUPOLE AND MAGNETIC DIPOLE MATRIX ELEMENTS

The *M1 5d<sub>3/2</sub>-5d<sub>5/2</sub>*, *5d<sub>3/2</sub>-6s* and *E2 5d<sub>3/2</sub>-5d<sub>5/2</sub>*, *5d<sub>j</sub>-6s* matrix elements are evaluated using the same approach as for the *E1* matrix elements. In Table VI, we list results for the magnetic dipole (*M1*) and electric quadrupole (*E2*) matrix elements calculated in different approximations: lowest-order DF, second-order RMBPT, third-order RMBPT, and all-order method with and without the triple excitations. The scaled all-order values are indicated by the label ‘‘sc.’’ Final recommended values and their uncertainties are given in the  $Z^{\text{final}}$  column. The last column gives relative uncertainties of the final values in %.

We combine recommended NIST energies [3] and our final values of the matrix elements listed in Table VI to calculate transition rates *A* given by

$$A(M1) = \frac{2.69735 \times 10^{13}}{(2J+1)\lambda^3} S(M1), \quad (2)$$

$$A(E2) = \frac{1.11995 \times 10^{18}}{(2J+1)\lambda^5} S(E2), \quad (3)$$

where the wavelength  $\lambda$  is in Å and the line strength  $S = Z^2$  is in atomic units. Transition rates *A* (in  $\text{s}^{-1}$ ) for the *M1 5d<sub>3/2</sub>-5d<sub>5/2</sub>* and *5d<sub>3/2</sub>-6s* transitions and the *E2 5d<sub>3/2</sub>-5d<sub>5/2</sub>*, *5d<sub>3/2</sub>-6s*, and *5d<sub>5/2</sub>-6s* transitions in  $\text{La}^{2+}$  are summarized in Table VII. The numbers in square brackets give the powers of 10. Final lifetimes of the *5d<sub>5/2</sub>* and *6s* levels are also given (in s). Uncertainties are given in parentheses for both transition rates and lifetimes.

The final value of the *M1 5d<sub>3/2</sub>-5d<sub>5/2</sub>* matrix element is almost the same as the lowest order DF result. The difference between the lowest-order and final all-order *5d<sub>3/2</sub>-5d<sub>5/2</sub>*

TABLE VI.  $E2$  and  $M1$  reduced matrix elements in Cs-like La III in atomic units calculated in different approximations. Absolute values are given. The lowest-order DF, second-order, third-order MBPT, and all-order SD and SDpT values are listed; the label “sc” indicates the scaled values. Final recommended values and their uncertainties are given in the  $Z^{\text{final}}$  column. The last column gives relative uncertainties of the final values in %.

Transition	$Z^{\text{DF}}$	$Z^{(\text{DF}+2)}$	$Z^{(\text{DF}+2+3)}$	$Z^{\text{SD}}$	$Z_{\text{sc}}^{(\text{SD})}$	$Z^{\text{SDpT}}$	$Z_{\text{sc}}^{\text{SDpT}}$	$Z^{\text{final}}$	Unc. (%)
Electric quadrupole transitions									
$5d_{3/2}-5d_{5/2}$	4.7651	4.7677	4.0210	4.1036	4.1142	4.1383	4.1066	4.1142	0.83
$5d_{3/2}-6s_{1/2}$	8.6130	8.6334	7.5129	7.7201	7.7502	7.8005	7.7368	7.7502	0.65
$5d_{5/2}-6s_{1/2}$	10.7812	10.8003	9.4490	9.6951	9.7294	9.7930	9.7131	9.7294	0.65
Magnetic dipole transitions									
$5d_{3/2}-5d_{5/2}$	1.5488	0.1549	1.5296	1.5492	1.5492	1.5492	1.5492	1.5492	0
$5d_{3/2}-6s_{1/2}$	1.007 [−5]	1.411 [−5]	1.333 [−2]	1.568 [−4]	1.564 [−4]	1.562 [−4]	1.566 [−4]	1.564 [−4]	0.38

transition rates is only 0.04%. The contribution of the  $E2$   $5d_{3/2}-5d_{5/2}$  transition to the  $5d_{5/2}$  lifetime is negligible and we find  $\tau(5d_{5/2}) = 14.99$  s, which is nearly the same as the DF value.

The value of the  $M1$   $5d_{3/2}-6s$  matrix element is not zero due to relativistic effects; it is smaller than the value of the  $M1$   $5d_{3/2}-5d_{5/2}$  matrix element by five orders of magnitude, as expected. The  $M1$  matrix element for the  $5d_{3/2}-6s$  transition changes substantially with the inclusion of the correlations, and correlation correction is actually larger than the DF value. This value is extremely sensitive to the treatment of the correlation correction. Our procedure for estimating the uncertainty described in [23] cannot be applied to this matrix element since different correlation corrections dominate for this transition. However, the contribution of the  $M1$   $5d_{3/2}-6s$  transition to the  $6s$  lifetime is negligible.

For all three  $E2$  transitions considered here, a single correlation correction term that can be improved by the scaling strongly dominates. Therefore, we can use the uncertainty estimate procedure described in [23].

## V. STATIC MULTIPOLE POLARIZABILITIES OF THE $6s$ STATE

The static multipole polarizability  $\alpha^{Ek}$  of Cs-like La III in its  $6s$  state can be separated into three terms: a dominant first term from intermediate valence excited states, ionic core contribution, and a small counter valence-core (VC) contribution term compensating for excitations from the core to the valence shell which violate the Pauli principle. The

TABLE VII.  $M1$  and  $E2$  transition rates  $A$  (in  $\text{s}^{-1}$ ) and  $6s$  and  $5d_{5/2}$  lifetimes  $\tau$  (in s) in Cs-like La III. Uncertainties are given in parentheses; numbers in brackets represent powers of 10.

	DF	Final
$A^{E2}(5d_{3/2}-5d_{5/2})$	4.49 [−6]	3.35(6) [−6]
$A^{M1}(5d_{3/2}-5d_{5/2})$	6.666 [−2]	6.669(0) [−2]
$\tau(5d_{5/2})$	15.00	14.99
$A^{M1}(5d_{3/2}-6s_{1/2})$	3.43 [−9]	8.32(8) [−7]
$A^{E2}(5d_{3/2}-6s_{1/2})$	1.93	1.56(2)
$A^{E2}(5d_{5/2}-6s_{1/2})$	1.61	1.31(2)
$\tau(6s_{1/2})$	0.283	0.348(4)

ionic core term is smaller than the valence one by several orders of magnitude and is evaluated here in the random-phase approximation (RPA) [26]. The term “VC” is also evaluated in the RPA; it contributes 0.55% to the  $E1$  polarizability.

The dominant valence contribution is calculated using the sum-over-state approach:

$$\alpha_v^{Ek} = \frac{1}{2k+1} \sum_n \frac{|\langle nl_j \| r^k C_{kq} \| 6s \rangle|^2}{E_{nl_j} - E_{6s}}, \quad (4)$$

where  $nl_j$  is  $np_j$ ,  $nd_j$ , and  $nf_j$  for  $k = 1, 2$ , and  $3$ , respectively [27], and  $C_{kq}(\hat{r})$  is a normalized spherical harmonic. The reduced matrix elements that give the dominant contributions to the above sum are evaluated using our final recommended values of the matrix elements and NIST energies [3]. The final values for the quadrupole and octupole matrix elements and their uncertainties are determined using the same procedure as for the dipole matrix elements. The uncertainties in the polarizability contributions are twice the uncertainties in the corresponding matrix elements.

Contributions to dipole, quadrupole, and octupole polarizabilities of the  $6s$  ground state are presented in Table VIII. The sum over states converges extremely well in this case, and the first two terms contribute 99.5% of the valence electric dipole polarizability. In the case of  $\alpha^{E2}$ , the contributions of the  $5d$  and  $6d$  states strongly cancel. The remaining 7.0% of valence electric quadrupole polarizability comes from the  $(7-26)nd$  states, which indicates much slower convergence of the sum over states than in the electric dipole case. The cancellation of contribution from the  $4f$  and  $5f$  states for the octupole polarizability is also important. The  $5f$  contribution is substantially larger than that of the  $4f$  states. The remaining 2.6% of  $\alpha^{E3}$  contributions are from the  $(6-26)nf$  states. Therefore, while the contribution of the first few terms in the sum over states dominates, the remaining contributions from the highly excited states have to be treated accurately as well for the electric quadrupole and electric-octupole polarizabilities.

We use recommended energies from [3] and our final matrix elements to evaluate terms in the sum with  $n \leq 13$ , and we use theoretical SD energies and matrix elements to evaluate terms with  $13 \leq n \leq 26$ . The remaining contributions to  $\alpha^{Ek}$  from orbitals with  $27 \leq n \leq 70$  are evaluated in the RPA approximation since the contributions from these terms are smaller than 0.01% in all cases. These terms are grouped

TABLE VIII. Contributions to multipole polarizabilities of the 6s state of Cs-like La III in  $a_0^3$ . Uncertainties are given in parentheses.

Contr.	$\alpha^{E1}$
6p <sub>1/2</sub>	19.90(11)
6p <sub>3/2</sub>	35.82(51)
(7-26)p <sub>j</sub>	0.27(0)
Tail	0.00
Term VC	-0.35
Core	7.67
Total	63.3(5)
Contr.	$\alpha^{E2}$
5d <sub>3/2</sub>	-194.0(2.5)
6d <sub>3/2</sub>	114.1(3)
(7-26)d <sub>3/2</sub>	6.5(1)
5d <sub>5/2</sub>	-346.6(4.5)
6d <sub>5/2</sub>	166.5(3)
(7-26)d <sub>5/2</sub>	10.5(2)
Tail	0.01
Core	27.8
Total	-215(5)
Contr.	$\alpha^{E3}$
4f <sub>5/2</sub>	-559(57)
5f <sub>5/2</sub>	2955(30)
(6-26)f <sub>5/2</sub>	57(4)
4f <sub>7/2</sub>	-1033(109)
5f <sub>7/2</sub>	3932(38)
(6-26)f <sub>7/2</sub>	84(6)
Tail	8
Core	198
Total	5576(133)

together as ‘‘Tail.’’ We evaluate core contributions in the random-phase approximation [26] for  $E1$ ,  $E2$ , and  $E3$ . Our result for core  $E1$  polarizability is the same as in [26]. The core polarizabilities are small in comparison with the valence ones and their uncertainties are negligible. We note that VC terms are zero for the  $E2$  and  $E3$  polarizabilities since the Cs-like La III core contains no  $nd$  or  $nf$  states.

## VI. SCALAR AND TENSOR EXCITED-STATE POLARIZABILITIES

The valence scalar  $\alpha_0(v)$  and tensor  $\alpha_2$  polarizabilities of an excited-state  $v$  of Cs-like La III are given by

$$\alpha_0(v) = \frac{2}{3(2j_v + 1)} \sum_{nlj} \frac{|\langle v || r C_1 || nlj \rangle|^2}{E_{nlj} - E_v}, \quad (5)$$

$$\alpha_2 = (-1)^{j_v} \sqrt{\frac{40j_v(2j_v - 1)}{3(j_v + 1)(2j_v + 1)(2j_v + 3)}} \times \sum_{nlj} (-1)^j \begin{Bmatrix} j_v & 1 & j \\ 1 & j_v & 2 \end{Bmatrix} \frac{|\langle v || r C_1 || nlj \rangle|^2}{E_{nlj} - E_v}. \quad (6)$$

The excited-state polarizability calculations are carried out in the same way as the calculations of the multipole polarizabilities discussed in the previous section.

TABLE IX. The  $\alpha_0(nlj)$  scalar and  $\alpha_2(nlj)$  tensor polarizabilities for Cs-like La III ion in  $a_0^3$ . Uncertainties are given in parentheses.

$nlj$	$\alpha_0(nlj)$	$\alpha_2(nlj)$
7s <sub>1/2</sub>	557(3)	
8s <sub>1/2</sub>	2779(9)	
9s <sub>1/2</sub>	10 058(9)	
10s <sub>1/2</sub>	29 502(16)	
6p <sub>1/2</sub>	19.7(4)	
7p <sub>1/2</sub>	-142(4)	
8p <sub>1/2</sub>	-1386(19)	
9p <sub>1/2</sub>	-6629(102)	
6p <sub>3/2</sub>	30.4(4)	6.0(3)
7p <sub>3/2</sub>	-37.7(3.8)	106(2)
8p <sub>3/2</sub>	-819(19)	632(6)
9p <sub>3/2</sub>	-4342(143)	2502(31)
5d <sub>3/2</sub>	25.5(5)	-6.1(1)
6d <sub>3/2</sub>	405.3(4.6)	-142( 1)
7d <sub>3/2</sub>	2864(22)	-992( 9)
8d <sub>3/2</sub>	12 453(71)	-4294(23)
9d <sub>3/2</sub>	41 030(240)	-14 067(68)
5d <sub>5/2</sub>	25.5(5)	-8.3(2)
6d <sub>5/2</sub>	405.1(4.8)	-184(2)
7d <sub>5/2</sub>	2865(22)	-1282(11)
8d <sub>5/2</sub>	12 412(78)	-5487(45)
9d <sub>5/2</sub>	40 930(260)	-18 080(120)
4f <sub>5/2</sub>	1.7(3)	5.0(3)
5f <sub>5/2</sub>	-41.8(4.4)	107(3)
6f <sub>5/2</sub>	-33 830(430)	12 780(150)
7f <sub>5/2</sub>	-164 500(1700)	61 870(610)
8f <sub>5/2</sub>	-601 300(10800)	225 100(3900)
4f <sub>7/2</sub>	1.4(4)	6.5(4)
5f <sub>7/2</sub>	-49.0(4.8)	134(4)
6f <sub>7/2</sub>	-25 090(310)	11 320(150)
7f <sub>7/2</sub>	-122 300(1200)	54 800(580)
8f <sub>7/2</sub>	-423 200(7600)	189 500(3600)

We list the contributions to the scalar polarizabilities of the  $ns$  ( $n = 7-10$ ),  $np$  ( $n = 6-9$ ),  $nd$  ( $n = 5-9$ ), and  $nf$  ( $n = 4-8$ ) states and tensor polarizabilities of the  $np_{3/2}$  ( $n = 6-9$ ),  $nd$  ( $n = 5-9$ ), and  $nf$  ( $n = 4-8$ ) states in Table IX. Uncertainties are given in parentheses.

The polarizability values rapidly increase with increasing  $n$ , but the rate of increase depends on  $l$ . The ratio of the  $\alpha_0(8l)$  and  $\alpha_0(7l)$  is substantially different for  $l = s$  and  $l = p$ . This difference in ratios decreases with  $n$ . The ratio of the  $\alpha_0(8s)$  and  $\alpha_0(7s)$  is equal to 5.0, while the ratio of the  $\alpha_0(8p)$  and  $\alpha_0(7p)$  is 9.7. The ratio of the  $\alpha_0(9s)$  and  $\alpha_0(8s)$  is equal to 3.6, while the ratio of the  $\alpha_0(9p)$  and  $\alpha_0(8p)$  is only slightly different (4.7).

The ratios of the  $\alpha_0(nl)$  and  $\alpha_0[(n-1)l]$  are similar for the  $nd_{3/2}$  states: 15.9, 7.1, 4.3, and 3.3 for  $n = 6, 7, 8$ , and 9, respectively; it is only different for tensor polarizabilities with  $n = 6$  (23.3, 7.0, 4.3, and 3.3). The values of  $\alpha_2(nd)$  and  $\alpha_0(nd)$  polarizabilities have different sign and their ratios are about 4.

The values of  $\alpha_0(4f)$  and  $\alpha_0(5f)$  have different signs and their ratio is equal -24.5. We note that with increasing  $n$  the

ratios of the  $\alpha_0(nf)$  and  $\alpha_0[(n-1)f]$  become similar to the ratios for the  $nd$  states. The values of the  $\alpha_0(nf)$  and  $\alpha_2(nf)$  have different signs for all states except the  $4f$  states. The ratio of values of the  $\alpha_0(nf)$  and  $\alpha_2(nf)$  changes from 0.34 and 0.39 for  $n = 4$  and 5 up to 2.6, 2.7, and 2.7 for  $n = 6, 7,$  and 8. The substantial change of ratios is due to large cancellation of different contributions especially for the states with  $n = 4$  and 5. We illustrated such cancellation for  $E2$  and  $E3$  multiple polarizabilities in Table VIII.

Significant cancellations among different contributions are found for the  $\alpha_0(6p_{3/2})$  and  $\alpha_0(7p_{3/2})$  polarizabilities. These cancellations were previously observed for  $\alpha_0(nl)$  and  $\alpha_2(nl)$  polarizabilities in  $\text{Sc}^{2+}$  [23],  $\text{Y}^{2+}$  [20], and  $\text{Th}^{3+}$  [28].

## VII. CONCLUSION

In summary, we carried out a systematic high-precision relativistic study of Cs-like La III atomic properties for the  $ns$ ,  $np$ ,  $nd$ ,  $nf$ , and  $ng$  ( $n \leq 9$ ) states using an all-order approach and evaluated uncertainties of our recommended values. The theoretical energy values are in excellent agreement with existing experimental data. Reduced matrix elements, oscillator strengths, transition rates, and lifetimes for the first low-lying levels up to  $n = 9$  are calculated. Electric dipole

( $6s-np$ ,  $n = 6-26$ ), electric quadrupole ( $6s-nd$ ,  $n = 5-26$ ), and electric-octupole ( $6s-nf$ ,  $n = 4-26$ ) matrix elements are calculated to obtain the ground-state  $E1$ ,  $E2$ , and  $E3$  static polarizabilities. Scalar polarizabilities of the  $ns$  ( $n = 7-10$ ),  $np$  ( $n = 6-9$ ),  $nd$  ( $n = 5-9$ ), and  $nf$  ( $n = 4-8$ ) states and tensor polarizabilities of the  $np_{3/2}$  ( $n = 6-9$ ),  $nd$  ( $n = 5-9$ ), and  $nf$  ( $n = 4-8$ ) states of Cs-like  $\text{La}^{2+}$  are evaluated. Particular care was taken to accurately treat contributions from highly excited states. The uncertainties are evaluated for most of the values listed in this work. This work provides recommended values critically evaluated for their accuracy for a number of atomic properties via a systematic high-precision study for use in astrophysics applications, theoretical modeling, and planning and analysis of various experiments that may utilize an interesting structure of La III levels with metastable  $5d_{5/2}$  and  $6s$  levels. This work also provides a benchmark test of the theoretical accuracy in lanthanide ions for recent proposals to develop ultra-accurate atomic clocks with highly charged lanthanide ions.

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- [1] R. C. Gibbs and H. E. White, *Phys. Rev.* **33**, 157 (1929).
  - [2] R. C. Gibbs and G. K. Schoepfle, *Phys. Rev.* **45**, 221 (1934).
  - [3] A. Kramida, Yu. Ralchenko, J. Reader, and NIST ASD Team (2012), NIST Atomic Spectra Database (ver. 5.0) [online], <http://physics.nist.gov/asd> [24 June 2013], National Institute of Standards and Technology, Gaithersburg, MD.
  - [4] W. C. Martin, R. Zalubas, and L. Hagan, in *Atomic Energy Levels - The Rare-Earth Elements*, *Natl. Stand. Ref. Data Ser., Natl. Bur. Stand.* (U.S. Government Printing Office, Washington, 1978), No. 60.
  - [5] A. Lindgård and S. E. Nielsen, *At. Data Nucl. Data Tables* **19**, 533 (1977).
  - [6] J. Migdalek and W. E. Baylis, *J. Quant. Spectrosc. Radiat. Transfer* **22**, 127 (1979).
  - [7] J. Migdalek and M. Wyrozumska, *J. Quant. Spectrosc. Radiat. Transfer* **37**, 581 (1987).
  - [8] R. D. Cowan, *The Theory of Atomic Structure and Spectra* (University of California, Berkeley, 1981).
  - [9] E. Biémont, Z. S. Li, P. Palmeri, and P. Quinet, *J. Phys. B* **32**, 3409 (1999).
  - [10] Z. S. Li and Jiang Zhankui, *Phys. Scr.* **60**, 414 (1999).
  - [11] E. Biémont and P. Quinet, *Phys. Scr.* **T105**, 38 (2003).
  - [12] P. Quinet and E. Biémont, *At. Data Nucl. Data Tables* **87**, 207 (2004).
  - [13] B. Karaçoban and L. Özdemir, *Cent. Eur. J. Phys.* **10**, 124 (2012).
  - [14] E. Eliav, S. Shmulyian, U. Kaldor, and Y. Ishikawa, *J. Chem. Phys.* **109**, 3954 (1998).
  - [15] V. A. Dzuba, A. Derevianko, and V. V. Flambaum, *Phys. Rev. A* **86**, 054502 (2012).
  - [16] M. S. Safronova, V. A. Dzuba, V. V. Flambaum, U. I. Safronova, and M. G. Kozlov (unpublished).
  - [17] M. S. Safronova and W. R. Johnson, in *Advances in Atomic, Molecular, and Optical Physics*, Vol. 55 (Academic Press, San Diego, 2008), pp. 191–233.
  - [18] M. S. Safronova, A. Derevianko, and W. R. Johnson, *Phys. Rev. A* **58**, 1016 (1998).
  - [19] M. S. Safronova, W. R. Johnson, and A. Derevianko, *Phys. Rev. A* **60**, 4476 (1999).
  - [20] U. I. Safronova and M. S. Safronova, *Phys. Rev. A* **87**, 032502 (2013).
  - [21] W. R. Johnson, Z. W. Liu, and J. Sapirstein, *At. Data and Nucl. Data Tables* **64**, 279 (1996).
  - [22] M. S. Safronova and U. I. Safronova, *Phys. Rev. A* **83**, 052508 (2011).
  - [23] M. S. Safronova and U. I. Safronova, *Phys. Rev. A* **85**, 022504 (2012).
  - [24] U. I. Safronova, *Phys. Rev. A* **81**, 052506 (2010).
  - [25] I. M. Savukov and W. R. Johnson, *Phys. Rev. A* **62**, 052506 (2000).
  - [26] W. R. Johnson, D. Kolb, and K.-N. Huang, *At. Data Nucl. Data Tables* **28**, 333 (1983).
  - [27] W. R. Johnson, D. R. Plante, and J. Sapirstein, *Adv. Atom. Mol. Opt. Phys.* **35**, 255 (1995).
  - [28] M. S. Safronova and U. I. Safronova, *Phys. Rev. A* **87**, 062509 (2013).