

Relativistic many-body calculation of energies, lifetimes, polarizabilities, blackbody radiative shift, and hyperfine constants in Lu^{2+}

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Energy levels of 30 low-lying states of Lu^{2+} and allowed electric-dipole matrix elements between these states are evaluated using a relativistic all-order method in which all single, double, and partial triple excitations of Dirac-Fock wave functions are included to all orders of perturbation theory. Matrix elements are critically evaluated for their accuracy and recommended values of the matrix elements are given together with uncertainty estimates. Line strengths, transition rates, and lifetimes of the metastable $5d_{3/2}$ and $5d_{5/2}$ states are calculated. Recommended values are given for static polarizabilities of the $6s$, $5d$, and $6p$ states and tensor polarizabilities of the $5d$ and $6p_{3/2}$ states. Uncertainties of the polarizability values are estimated in all cases. The blackbody radiation shift of the $6s_{1/2}$ – $5d_{5/2}$ transition frequency of the Lu^{2+} ion is calculated with the aid of the recommended scalar polarizabilities of the $6s_{1/2}$ and $5d_{5/2}$ states. Finally, A and B hyperfine constants are determined for states of $^{175}\text{Lu}^{2+}$ with $n \leq 9$. This work provides recommended values of transition matrix elements, polarizabilities, and hyperfine constants of Lu^{2+} , critically evaluated for accuracy, for benchmark tests of high-precision theoretical methodology and planning of future experiments.

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I. INTRODUCTION

The development of high-precision optical atomic clocks is important for many applications [1], including precision timekeeping, tracking of deep-space probes, study of many-body quantum systems [2], relativistic geodesy with potential future application to monitor volcanic magma chambers and earthquake prediction [3], and tests of fundamental physics such as search for variation of fundamental constants [4,5], tests of Lorentz invariance [6], and search for topological dark matter [7].

While trapped ion clocks achieved the ultralow uncertainty of 3×10^{-18} , realized with the octupole transition in Yb^+ [8], a significant bottleneck to further improvement of the accuracy arises from the relatively low stability achievable with a single ion [1]. Recently, singly ionized lutetium has been proposed as a possible candidate to overcome this hurdle via the use of large ion crystals with a special scheme to cancel the effect of micromotion [9,10]. The crucial condition for the implementation of such a scheme is the negative value of the scalar polarizability difference for the clock transition [9–13].

Doubly ionized lutetium is another system that satisfies such a condition and is a potentially promising candidate for multi-ion clock development [13]. Clock considerations for Lu^{2+} were discussed in [13], including the prospects for suppression of clock shifts. In this work, we study relevant parameters of Lu^{2+} , including transition matrix elements,

lifetimes, polarizabilities, hyperfine constants, and the blackbody radiation (BBR) shift of the potential clock transition.

The properties of neutral, singly ionized, and doubly ionized lutetium were investigated recently in Refs. [10,13–16]. Dzuba *et al.* [14] evaluated excitation energies, ionization potentials, and static dipole polarizabilities of lutetium using a combination of the configuration interaction method and the all-order single-double coupled-cluster technique. The calculations in [14] included Breit and quantum electrodynamic corrections. Dzuba [15] calculated the excitation energies of the lowest states of Lu^+ and Lu^{2+} using a simplified version of the method used in [14] but leading to results of comparable accuracy. Kozlov *et al.* [16] studied a wide range of neutral atoms and ions suitable for ultraprecise atomic optical clocks, in which the BBR shifts of the clock transition frequencies are naturally suppressed and presented calculations of the BBR shift in Lu^+ . Atomic properties of Lu^+ were investigated by Paez *et al.* [10], where a joint experimental and theoretical investigation of Lu^+ as a clock candidate was reported and measurements relevant to practical clock operation were made. Calculations of scalar and tensor polarizabilities for clock states over a range of wavelengths were also given in [10]. Arnold and Barrett [13] show that Lu^{2+} is among the clock candidates with an upper D state for which shifts from rank 2 tensor interactions can be practically eliminated by operating at a judiciously chosen field-insensitive transition.

Early publications include only a few experimental [17,18] and theoretical [19–22] studies of Lu^{2+} . The one-electron spectrum of Lu^{2+} was studied by Kaufman and Sugar.

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The ns series was used to derive an ionization energy of $169\,049 \pm 10 \text{ cm}^{-1}$. The ground-state hyperfine constant was measured in the same work [17]. Subsequently, $5f - ng$ ($n = 5, 6$) lines and ng levels of Lu^{2+} were reported by Kaufman and Sugar [18]. Migdalek [19] reported calculations of relativistic model-potential ionization energies and transition probabilities in the one-electron spectrum of doubly ionized lutetium employing a technique that includes valence-core exchange and correlation. The influence of polarization of the core by the valence electron on ionization energies and transition probabilities was also studied in [19]. Relativistic ionization energies and fine-structure intervals of $4f^{14}nl$ states in Lu^{2+} ion were computed by Koc and Migdalek [20]. Weighted oscillator strengths and radiative transition probabilities of Lu^{2+} were evaluated by Biémont *et al.* [21] using the relativistic Hartree-Fock technique described by Cowan (1981), in which core-polarization effects are incorporated. Quinet and Biémont [22] calculated the Landé g factor for over 1500 energy levels of doubly ionized lanthanides ($Z = 57-71$) using the relativistic Hartree-Fock method combined with

a least-squares fit of the eigenvalues to observed energy levels; the resulting energies were compared with previous experimental and theoretical values.

In the present work, a relativistic all-order method is used to calculate properties of the first 30 excited ns , np , nd , and nf states of Lu^{2+} . Electric-dipole matrix elements for allowed transitions between low-lying $6s-6p$, $6p-6d$, $6d-6f$, and $5d-5f$ states of Lu^{2+} are calculated and recommended values are given for the electric-dipole matrix elements. Line strengths, transition rates, and lifetimes are calculated for the metastable $5d_{3/2}$ and $5d_{5/2}$ states. Scalar and tensor polarizabilities of the $6s$, $5d$, and $6p$ states are evaluated and recommended values of the polarizabilities are given together with uncertainties in these values. Results for static scalar polarizabilities of the $6s_{1/2}$ ground and $5d_{5/2}$ excited states are used to determine the BBR shift of the $6s_{1/2}-5d_{5/2}$ clock transition frequency of Lu^{2+} . Finally, we investigate the hyperfine structure of $^{175}\text{Lu}^{2+}$ and evaluate the hyperfine A and B constants for low-lying levels with principal quantum numbers $n \leq 9$.

TABLE I. Contributions to the energy levels of Lu^{2+} , in cm^{-1} : $E^{(0)}$ is the zeroth-order Dirac-Fock energy, $E^{(2)}$ and $E^{(3)}$ are the second- and third-order Coulomb correlation energies, E^{SD} and E^{SDpT} are the Coulomb correlation energies in the SD and SDpT approximations, $E_{\text{extra}}^{(3)}$ is the part of the third-order energy missing in the SD approximation, $E^{(l>6)}$ is the contribution to the second-order energy from partial waves with $l > 6$, and $B^{(1)}$ and $B^{(2)}$ are the first-order Breit and second-order Coulomb-Breit energies. The correlation energies are $E_{\text{corr}}^{(3)} = E^{(2)} + E^{(3)} + B^{(1)} + B^{(2)}$, $E_{\text{corr}}^{\text{SD}} = E^{\text{SD}} + E_{\text{extra}}^{(3)} + E^{(l>6)} + B^{(1)} + B^{(2)}$, and $E_{\text{corr}}^{\text{SDpT}} = E^{\text{SDpT}} + E^{(l>6)} + B^{(1)} + B^{(2)}$. Relative contributions to the correlation energy $E_{\text{corr}}/(E^{(0)} + E_{\text{corr}})$, in percentage, are listed in the last three columns.

nlj	$E^{(0)}$	$E^{(2)}$	$E^{(3)}$	E^{SD}	$E_{\text{extra}}^{(3)}$	E^{SDpT}	$E^{(l>6)}$	$B^{(1)}$	$B^{(2)}$	$E_{\text{corr}}^{(3)}$	$E_{\text{corr}}^{\text{SD}}$	$E_{\text{corr}}^{\text{SDpT}}$
$6s_{1/2}$	-160745	-10006	2041	-9005	340	-8627	-107	209	-354	4.8	5.2	5.2
$5d_{3/2}$	-152866	-11922	324	-10508	-1378	11288	-395	330	-905	7.4	7.8	7.4
$5d_{5/2}$	-150818	-10714	-53	-9534	-1434	10341	-371	244	-835	7.0	7.3	7.0
$6d_{3/2}$	-74377	-2585	258	-2307	-173	-2285	-69	71	-173	3.2	3.4	3.2
$6d_{5/2}$	-73679	-2445	204	-2207	-183	-2285	-67	54	-165	3.1	3.4	3.2
$7d_{3/2}$	-45329	-1150	137	-1042	-64	-1036	-29	32	-75	2.3	2.5	2.4
$7d_{5/2}$	-44994	-1101	116	-1007	-68	-1036	-29	24	-72	2.2	2.5	2.4
$8d_{3/2}$	-30630	-626	81	-580	81	-586	-15	17	-40	1.8	1.7	2.0
$8d_{5/2}$	-30442	-603	70	-566	70	-572	-15	13	-39	1.8	1.7	2.0
$9d_{3/2}$	-22105	-381	52	-360	52	-360	-9	10	-24	1.5	1.5	1.7
$9d_{5/2}$	-21990	-368	45	-353	45	-357	-9	8	-23	1.5	1.5	1.7
$7s_{1/2}$	-79912	-2972	608	-2596	85	-2510	-33	70	-114	2.9	3.1	3.1
$8s_{1/2}$	-48159	-1318	270	-1139	35	-1105	-15	33	-52	2.2	2.3	2.3
$9s_{1/2}$	-32240	-705	145	-608	18	-590	-8	18	-28	1.7	1.9	1.9
$6p_{1/2}$	-125045	-6161	1024	-5947	170	-5720	-60	179	-199	4.0	4.5	4.4
$6p_{3/2}$	-119552	-5171	767	-5024	87	-4873	-53	123	-181	3.6	4.1	4.0
$7p_{1/2}$	-66610	-2169	343	-2224	47	-2144	-22	70	-77	2.7	3.2	3.2
$7p_{3/2}$	-64459	-1884	269	-1929	22	-1871	-21	49	-72	2.5	2.9	2.9
$8p_{1/2}$	-41708	-1046	160	-985	22	-954	-11	35	-38	2.1	2.3	2.3
$8p_{3/2}$	-40635	-923	128	-622	128	-618	-10	25	-36	1.9	1.3	1.5
$9p_{1/2}$	-28623	-588	88	-439	12	-434	-6	20	-22	1.7	1.4	1.4
$9p_{3/2}$	-28010	-524	71	-403	6	-402	-6	14	-21	1.5	1.4	1.4
$5f_{5/2}$	-61961	-1546	258	-1880	258	-1694	-17	6	-24	2.1	2.6	2.7
$5f_{7/2}$	-61949	-1516	204	-1833	204	-1663	-17	5	-27	2.1	2.6	2.7
$6f_{5/2}$	-39685	-860	132	-589	132	-552	-12	4	-18	1.8	1.2	1.4
$6f_{7/2}$	-39676	-838	112	-388	112	-370	-12	4	-19	1.8	0.8	1.0
$7f_{5/2}$	-27558	-472	67	-468	36	-468	-8	3	-12	1.5	1.6	1.7
$7f_{7/2}$	-27551	-457	54	-435	31	-435	-8	2	-13	1.5	1.5	1.6
$8f_{5/2}$	-20241	-302	38	-302	22	-302	-5	2	-8	1.3	1.4	1.5
$8f_{7/2}$	-20236	-292	30	-282	19	-282	-5	2	-9	1.3	1.3	1.4

II. CORRELATION ENERGIES OF Lu III

Contributions to energies of Lu^{2+} are listed in Table I. These contributions include the zeroth-order Dirac-Fock energy $E^{(0)}$, relativistic second- and third-order many-body perturbation theory (MBPT) correlation energies $E^{(2)}$ and $E^{(3)}$, all-order energies in the single-double (SD) approximation E^{SD} , in which single and double excitations of the Dirac-Fock wave function are summed to all orders of perturbation theory, and all-order single-double partial triple (SDpT) energies E^{SDpT} , in which single, double, and the dominant class of triple excitations are summed to all orders. The SD energy E^{SD} includes $E^{(2)}$ completely but misses part of the third-order energy. The missing part $E_{\text{extra}}^{(3)}$ is included perturbatively in the total SD energy. The triple-excitation terms in the SDpT wave functions were originally discussed by Safronova *et al.* [23,24]; these terms automatically include the entire third-order energy and substantially improve the accuracy of the SD functions. The SDpT functions have been used in a number of publications [25–33] to evaluate multipole matrix elements.

As expected, the largest contribution to the correlation energy comes from the second-order term $E^{(2)}$. This term is relatively simple to calculate; thus, we calculate $E^{(2)}$ with a higher numerical accuracy than E^{SD} and E^{SDpT} , which are limited to partial waves with $l \leq 6$. The second-order energy $E^{(2)}$, by contrast, includes partial waves up to $l_{\text{max}} = 8$ and is extrapolated to account for contributions from higher partial waves (see, for example, [32] and [33]). In the column headed $E^{(l>6)}$ in Table I, we list the difference between the value of $E^{(2)}$ obtained with extrapolation and the value of $E^{(2)}$ evaluated with $l_{\text{max}} = 6$. The columns in Table I headed $B^{(1)}$

and $B^{(2)}$ list the first-order Breit energy and the second-order Breit-Coulomb energy, respectively.

The third-order, SD, and SDpT correlation energies are defined by $E_{\text{corr}}^{(3)} = E^{(2)} + E^{(3)} + B^{(1)} + B^{(2)}$, $E_{\text{corr}}^{\text{SD}} = E^{\text{SD}} + E_{\text{extra}}^{(3)} + E^{(l>6)} + B^{(1)} + B^{(2)}$, and $E_{\text{corr}}^{\text{SDpT}} = E^{\text{SDpT}} + E^{(l>6)} + B^{(1)} + B^{(2)}$. The relative correlation contributions $E_{\text{corr}}/(E^{(0)} + E_{\text{corr}})$ (in percentage) are given in the final three columns in Table I. Comparing the values listed in the last three columns, we find that the largest correlation contributions are for energies evaluated in the SDpT approximation. The largest correlation contributions (about 7%) are for the $5d_{3/2}$ and the $5d_{5/2}$ levels. The smallest ones (about 1.5%) are for the nf_j ($n = 6-8$) levels. For these levels the Breit corrections $B^{(1)}$ and $B^{(2)}$ are smaller than for other levels displayed in Table I. We do not list QED corrections, however, estimates of the QED corrections are included in the totals listed in Table II. The largest QED correction (30 cm^{-1}) is for the $6s$ level.

Recommended energies of states of Lu^{2+} from the National Institute of Standards and Technology (NIST) database [34] are given in the column in Table II headed E_{NIST} . This column is followed by theoretical removal energies $E_{\text{tot}}^{(3)} = E^{(0)} + E_{\text{corr}}^{(3)} + E^{(\text{QED})}$, $E_{\text{tot}}^{\text{SD}} = E^{(0)} + E_{\text{corr}}^{\text{SD}} + E^{(\text{QED})}$, and $E_{\text{tot}}^{\text{SDpT}} = E^{(0)} + E_{\text{corr}}^{\text{SDpT}} + E^{(\text{QED})}$. Relative differences (in percentage) between the theoretical third-order and all-order energies and the experimental data, $\delta E = (E_{\text{tot}} - E_{\text{NIST}})/E_{\text{NIST}}$, are given in the final three columns in Table II. The smallest differences are obtained using the SDpT method. Results for the $8d$, $9d$, $8p$, and $9p$ levels are not listed in Table II since these levels are not included in the NIST database [34].

TABLE II. The total removal energies (cm^{-1}) of Lu^{2+} [$E_{\text{tot}}^{(3)} = E^{(0)} + E_{\text{corr}}^{(3)} + E^{(\text{QED})}$, $E_{\text{tot}}^{\text{SD}} = E^{(0)} + E_{\text{corr}}^{\text{SD}} + E^{(\text{QED})}$, and $E_{\text{tot}}^{\text{SDpT}} = E^{(0)} + E_{\text{corr}}^{\text{SDpT}} + E^{(\text{QED})}$] are compared with the recommended NIST energies E_{NIST} [34]. The relative difference $\delta E = (E_{\text{tot}} - E_{\text{NIST}})/E_{\text{NIST}}$, in percentage, is listed in the last three columns.

nlj	E_{NIST}	$E_{\text{tot}}^{(3)}$	$E_{\text{tot}}^{\text{SD}}$	$E_{\text{tot}}^{\text{SDpT}}$	$\delta E^{(3)}$	δE^{SD}	δE^{SDpT}
$6s_{1/2}$	-169014	-168817	-169625	-169587	-0.12	0.36	0.34
$5d_{3/2}$	-163306	-165040	-165723	-165125	1.05	1.46	1.10
$5d_{5/2}$	-160366	-162177	-162748	-162122	1.12	1.46	1.08
$6d_{3/2}$	-76692	-76806	-77028	-76832	0.15	0.44	0.18
$6d_{5/2}$	-75906	-76031	-76247	-76141	0.16	0.45	0.31
$7d_{3/2}$	-46392	-46385	-46507	-46437	-0.01	0.25	0.10
$7d_{5/2}$	-46033	-46026	-46145	-46105	-0.01	0.24	0.16
$7s_{1/2}$	-82333	-82313	-82493	-82493	-0.02	0.19	0.19
$8s_{1/2}$	-49229	-49225	-49297	-49298	-0.01	0.14	0.14
$9s_{1/2}$	-32804	-32810	-32848	-32848	0.02	0.13	0.13
$6p_{1/2}$	-130613	-130202	-130902	-130844	-0.32	0.22	0.18
$6p_{3/2}$	-124309	-124014	-124599	-124536	-0.24	0.23	0.18
$7p_{1/2}$	-68657	-68443	-68816	-68783	-0.31	0.23	0.18
$7p_{3/2}$	-66203	-66097	-66409	-66374	-0.16	0.31	0.26
$5f_{5/2}$	-63423	-63268	-63619	-63691	-0.25	0.31	0.42
$5f_{7/2}$	-63310	-63283	-63617	-63651	-0.04	0.48	0.54
$6f_{5/2}$	-40214	-40427	-40168	-40262	0.53	-0.12	0.12
$6f_{7/2}$	-39961	-40418	-39980	-40074	1.13	0.05	0.28
$7f_{5/2}$	-27944	-27971	-28006	-28042	0.10	0.22	0.35
$7f_{7/2}$	-27922	-27964	-27973	-28004	0.15	0.18	0.29
$8f_{5/2}$	-20500	-20511	-20532	-20554	0.05	0.15	0.26
$8f_{7/2}$	-20484	-20506	-20512	-20530	0.11	0.14	0.23

TABLE III. Recommended values of reduced electric-dipole matrix elements (in a.u.). Lowest-order DF, all-order SD, and SDpT values are listed; the label “sc” indicates scaled values. Recommended values of the matrix elements are listed in the column headed “Final” and the corresponding uncertainties are listed under the heading “Unc.” The last column lists relative uncertainties (Rel. unc.), in percentage.

Transition	DHF	SD	SDsc	SDpT	SDpTsc	Final	Unc.	Rel. unc.
6s _{1/2} –6p _{1/2}	2.7279	2.3177	2.3264	2.3193	2.3236	2.3177	0.0087	0.38
6s _{1/2} –7p _{1/2}	0.0107	0.1716	0.1703	0.1716	0.1702	0.1716	0.0014	0.82
6s _{1/2} –8p _{1/2}	0.0339	0.1343		0.1359		0.1343	0.0016	1.20
6s _{1/2} –9p _{1/2}	0.0289	0.0398		0.0409		0.0398	0.0011	2.76
6s _{1/2} –6p _{3/2}	3.8241	3.2695	3.2826	3.2721	3.2786	3.2695	0.0131	0.40
6s _{1/2} –7p _{3/2}	0.2041	0.0225	0.0186	0.0237	0.0182	0.0225	0.0043	19.1
6s _{1/2} –8p _{3/2}	0.0658	0.0803		0.0838		0.0838	0.0035	4.15
6s _{1/2} –9p _{3/2}	0.0333	0.0099		0.0072		0.0099	0.0027	27.3
6p _{1/2} –6s _{1/2}	2.7279	2.3177	2.3260	2.3193	2.3236	2.3177	0.0083	0.36
6p _{1/2} –7s _{1/2}	1.6729	1.6315	1.6265	1.6240	1.6246	1.6265	0.0071	0.44
6p _{1/2} –8s _{1/2}	0.4753	0.4807	0.4803	0.4721	0.4723	0.4807	0.0117	2.43
6p _{1/2} –9s _{1/2}	0.2595	0.2678	0.2677	0.2590	0.2594	0.2678	0.0088	3.29
6p _{1/2} –5d _{3/2}	2.4588	2.0696	2.0701	2.0459	2.0598	2.0696	0.0343	1.66
6p _{1/2} –6d _{3/2}	3.6470	3.3671	3.3753	3.3876	3.3975	3.3671	0.0313	0.93
6p _{1/2} –7d _{3/2}	1.0403	0.9077	0.9049	0.9072	0.9040	0.9077	0.0032	0.35
6p _{3/2} –6s _{1/2}	3.8241	3.2695	3.2827	3.2721	3.2786	3.2695	0.0132	0.40
6p _{3/2} –7s _{1/2}	2.8163	2.7497	2.7413	2.7083	2.7081	2.7413	0.0469	1.71
6p _{3/2} –8s _{1/2}	0.7216	0.7151	0.7153	0.6860	0.6865	0.7153	0.0415	5.80
6p _{3/2} –9s _{1/2}	0.3857	0.3838	0.3843	0.3618	0.3625	0.3838	0.0318	8.29
6p _{3/2} –5d _{3/2}	1.0423	0.8898	0.8901	0.8788	0.8854	0.8898	0.0160	1.80
6p _{3/2} –6d _{3/2}	1.8135	1.6845	1.6876	1.6921	1.6958	1.6845	0.0113	0.67
6p _{3/2} –7d _{3/2}	0.4490	0.3845	0.3828	0.3835	0.3815	0.3845	0.0030	0.78
6p _{3/2} –5d _{5/2}	3.2482	2.7973	2.7962	2.7632	2.7826	2.7973	0.0467	1.67
6p _{3/2} –6d _{5/2}	5.3437	4.9661	4.9766	4.9900	4.9928	4.9661	0.0228	0.46
6p _{3/2} –7d _{5/2}	1.3809	1.1953	1.1892	1.1922	1.1896	1.1953	0.0057	0.48
5d _{3/2} –6p _{1/2}	2.4588	2.0696	2.0694	2.0459	2.0598	2.0696	0.0332	1.60
5d _{3/2} –7p _{1/2}	0.2751	0.1094	0.1174	0.1159	0.1133	0.1094	0.0080	7.31
5d _{3/2} –8p _{1/2}	0.1487	0.0905		0.0941		0.0905	0.0036	3.98
5d _{3/2} –9p _{1/2}	0.1006	0.0709		0.0729		0.0709	0.0020	2.82
5d _{3/2} –6p _{3/2}	1.0423	0.8898	0.8897	0.8788	0.8854	0.8898	0.0155	1.74
5d _{3/2} –7p _{3/2}	0.1530	0.0924	0.0959	0.0951	0.0951	0.0924	0.0035	3.79
5d _{3/2} –8p _{3/2}	0.0819	0.0728		0.0735		0.0728	0.0007	0.96
5d _{3/2} –9p _{3/2}	0.0550	0.0420		0.0425		0.0420	0.0005	1.19
5d _{5/2} –6p _{3/2}	3.2482	2.7973	2.7953	2.7632	2.7826	2.7973	0.0454	1.62
5d _{5/2} –7p _{3/2}	0.4451	0.2694	0.2814	0.2794	0.2795	0.2694	0.0120	4.45
5d _{5/2} –8p _{3/2}	0.2382	0.2246		0.2300		0.2246	0.0054	2.40
5d _{5/2} –9p _{3/2}	0.1601	0.1297		0.1317		0.1297	0.0020	1.54
5d _{3/2} –5f _{5/2}	2.5512	2.0403	2.0057	1.9972	1.9979	2.0403	0.0431	2.11
5d _{3/2} –6f _{5/2}	1.3900	1.2302	1.2303	1.2221	1.2274	1.2302	0.0117	0.95
5d _{3/2} –7f _{5/2}	0.9226	0.7511	0.7529	0.7464	0.7494	0.7511	0.0065	0.86
5d _{3/2} –8f _{5/2}	0.6769	0.5406	0.5427	0.5361	0.5380	0.5406	0.0066	1.22
5d _{5/2} –5f _{5/2}	0.7099	0.5853	0.5754	0.5733	0.5734	0.5853	0.0099	1.69
5d _{5/2} –6f _{5/2}	0.3816	0.3369	0.3368	0.3348	0.3361	0.3369	0.0029	0.86
5d _{5/2} –7f _{5/2}	0.2518	0.2021	0.2027	0.2010	0.2018	0.2021	0.0017	0.84
5d _{5/2} –8f _{5/2}	0.1842	0.1441	0.1447	0.1430	0.1435	0.1441	0.0017	1.18
5d _{5/2} –5f _{7/2}	3.1693	2.5743	2.5256	2.5224	2.5161	2.5743	0.0582	2.26
5d _{5/2} –6f _{7/2}	1.7028	1.5869	1.5889	1.5806	1.5876	1.5889	0.0083	0.52
5d _{5/2} –7f _{7/2}	1.1235	0.9305	0.9326	0.9253	0.9287	0.9305	0.0073	0.78
5d _{5/2} –8f _{7/2}	0.8218	0.6669	0.6693	0.6644	0.6665	0.6669	0.0049	0.73

III. ELECTRIC-DIPOLE MATRIX ELEMENTS AND LIFETIMES

In Table III, recommended values of reduced electric dipole matrix elements of 49 $6s\text{-}np$, $6p\text{-}ns$, $6p\text{-}nd$, $5d\text{-}np$, and $5d\text{-}nf$ transitions are presented. The absolute values in atomic units ($e a_0$) are given in all cases. Matrix elements for eight $6s\text{-}np$ ($n = 6\text{-}9$) transitions, eight $6p\text{-}ns$ ($n = 6\text{-}9$) transitions, nine $6p\text{-}nd$ ($n = 5\text{-}7$) transitions, twelve $5d\text{-}np$ ($n = 6\text{-}9$) transitions, and twelve $5d\text{-}nf$ ($n = 5\text{-}8$) transitions are evaluated. The recommended values of the matrix elements for these transitions are listed in the column headed “Final.” To determine these values and estimate the corresponding uncertainties, we carried out a series of calculations using different methods of increasing accuracy: lowest-order DF, second-order MBPT, third-order MBPT, and all-order methods. MBPT calculations were carried out using the method described in Ref. [35]. Comparisons of values obtained in different approximations allow us to evaluate the size of the second-, third-, and higher-order correlation corrections as well as estimate uncertainties in the final values. The evaluation of the uncertainty of the matrix elements using this approach was described in detail in Refs. [30] and [36]. The uncertainty evaluation is based on four all-order calculations. These include two *ab initio* all-order calculations, carried out with and without the partial triple excitations, and two calculations that included semiempirical estimates of high-order correlation corrections starting from both *ab initio* runs. We use the differences in these four values to estimate the uncertainty in the final results for each transition. The estimates are based on an algorithm that accounted for the dominant contributions.

The column labeled “Rel. unc.” in Table III lists the relative uncertainties of the final reduced matrix elements (in percentage). We could not carry out the scaling for the $8d$, $9d$, $8p$, and $9p$ levels since there are no experimental energy values available. As a result, we used only the SD and SDpT values to determine the uncertainties listed in the last two columns in Table III. Uncertainties listed in the column “Rel. unc.” in Table III are in the range 0.38%–2%. However, there are matrix elements with uncertainties equal to 19% and 27%. Such large uncertainties occur only for very small matrix elements, 0.0225 and 0.0099, respectively, where the relative contribution of correlation corrections is very large. Uncertainties for larger matrix elements, such as the $6s\text{-}6p$ matrix element, are much smaller (0.38% and 0.40%). Uncertainties in matrix elements of $5d\text{-}nf$ transitions are smaller than those of the $5d\text{-}np$ transitions.

Line strengths S (a.u.), transition rates A (s^{-1}), and lifetimes τ (s) of the metastable $5d$ states of the Lu^{2+} ion, evaluated by the scaled SD method, are listed in Table IV.

IV. SCALAR AND TENSOR EXCITED-STATE POLARIZABILITIES

The scalar $\alpha_0(v)$ and tensor $\alpha_2(v)$ polarizabilities of an excited state with one valence electron v are given by

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

TABLE IV. Multipolarities (MP), wavelengths λ (\AA), line strengths S (a.u.), transition rates A (s^{-1}) and lifetimes τ (s) are given for transitions between metastable $5d_{3/2}$ and $5d_{5/2}$ states and the $6s_{1/2}$ ground state of Lu^{2+} . Numbers in brackets represent powers of 10.

Transition	MP	λ (\AA)	S (a.u.)	A (s^{-1})	τ (s)
$5d_{3/2}\text{-}6s_{1/2}$	$E2$	17520	37.831	6.415 [−3]	155.9
$5d_{3/2}\text{-}6s_{1/2}$	$M1$	17520	1.39 [−7]	1.744 [−7]	
$5d_{5/2}\text{-}5d_{3/2}$	$M1$	34011	2.4013	2.744 [−1]	3.029
$5d_{5/2}\text{-}6s_{1/2}$	$E2$	11564	61.234	5.527 [−2]	
$5d_{5/2}\text{-}5d_{3/2}$	$E2$	34011	12.016	4.928 [−4]	

and

$$\alpha_2(v) = (-1)^{j_v} \sqrt{\frac{40j_v(2j_v - 1)}{3(j_v + 1)(2j_v + 1)(2j_v + 3)}} \times \sum_{nlj} (-1)^j \begin{Bmatrix} j_v & 1 & j \\ 1 & j_v & 2 \end{Bmatrix} \frac{|\langle v || r C_2 || nlj \rangle|^2}{E_{nlj} - E_v}, \quad (2)$$

where $C_{kq}(\hat{r})$ is a normalized spherical harmonic and where the indices nlj in the sums range over np_j , nd_j , and nf_j .

The polarizabilities in Eqs. (1) and (2) can be separated into two parts: a dominant term from intermediate valence-excited states and a contribution from core-excited states. The second term is smaller than the former by several orders of magnitude and is evaluated here in the random-phase approximation [37]. The dominant valence contribution is calculated using the sum-over-state approach using our theoretical recommended values of the matrix elements and energies from the NIST database [34]. Uncertainties in the polarizability contributions are obtained from the uncertainties in the corresponding matrix elements.

Contributions to the scalar polarizabilities of the $6s_{1/2}$ state of Lu^{2+} are listed in Table V. The corresponding uncertainty is given in parentheses. The $6s_{1/2}\text{-}6p_{1/2}$ and $6s_{1/2}\text{-}6p_{3/2}$ transitions account for 99.7% of the final value of $\alpha_0(6s_{1/2})$.

TABLE V. Contributions to scalar polarizabilities of the $6s$ state of Lu^{2+} , in units of a_0^3 . The dominant contributions are listed separately, with the corresponding absolute values of electric-dipole reduced matrix elements listed in the column labeled D . The experimental [34] transition energies are given in the column ΔE . Uncertainties are given in parentheses.

Contribution	ΔE	D	$\alpha_0^{E1}(6s)$
$6p_{1/2}$	38400.61	2.3177	10.234(78)
$7p_{1/2}$	100357.09	0.1716	0.021(0)
$(8\text{-}26)p_{1/2}$			0.014(0)
$6p_{3/2}$	44705.21	3.2695	17.493(140)
$7p_{3/2}$	102810.82	−0.0225	0.00(0)
$(8\text{-}26)p_{3/2}$			0.034(0)
Core			4.265 (080)
Term-vc			−0.678(0)
Tail			0.00
Total			31.91(18)

TABLE VI. Contributions to the scalar and tensor polarizabilities of the $5d_{3/2}$ and $5d_{5/2}$ states of Lu^{2+} in a_0^3 . Uncertainties are given in parentheses.

Contribution	$\alpha_0(5d_{3/2})$	$\alpha_2(5d_{3/2})$	Contribution	$\alpha_0(5d_{5/2})$	$\alpha_2(5d_{5/2})$
$6p_{1/2}$	4.792(153)	-4.792(153)	$6p_{3/2}$	5.292(171)	-5.292(171)
$7p_{1/2}$	0.005(1)	-0.005(1)	$7p_{3/2}$	0.019(2)	-0.019(2)
$(8-26)p_{1/2}$	0.003(0)	-0.003(0)	$(9-26)p_{3/2}$	0.015(0)	-0.015(0)
$6p_{3/2}$	0.743(26)	0.594(21)	$5f_{5/2}$	0.086(3)	0.098(3)
$7p_{3/2}$	0.003(0)	0.003(0)	$6f_{5/2}$	0.023(0)	0.026(0)
$(9-26)p_{3/2}$	0.000(0)	0.001(0)	$7f_{5/2}$	0.009(0)	0.008(0)
			$8f_{5/2}$	0.089(1)	0.078(1)
			$(9-26)f_{5/2}$	0.002(0)	0.005(0)
$5f_{5/2}$	1.525(64)	-0.305(13)	$5f_{7/2}$	1.665(75)	-0.595(27)
$6f_{5/2}$	0.450(9)	-0.090(2)	$6f_{7/2}$	0.511(5)	-0.183(2)
$7f_{5/2}$	0.152(3)	-0.030(1)	$7f_{7/2}$	0.159(2)	-0.057(1)
$8f_{5/2}$	0.075(2)	-0.015(0)	$8f_{7/2}$	0.078(1)	-0.028(0)
$9f_{5/2}$	0.043(0)	-0.009(0)	$9f_{7/2}$	0.044(0)	-0.016(0)
$(10-26)f_{5/2}$	0.181(0)	-0.037(0)	$(10-26)f_{7/2}$	0.169(0)	-0.048(0)
Core	4.264(080)	0.0	Core	4.264(080)	0.0
Term-vc	-0.261	0.0	Term-vc	-0.355(0)	0.0
Tail	0.0	0.0	Tail	0.0	0.0
Total	11.98(19)	-4.69(15)	Total	12.09(20)	-6.03(17)

Contributions to the scalar and tensor polarizabilities of the $5d_{3/2}$ and $5d_{5/2}$ levels of Lu^{2+} are given in Table VI. The largest contribution to $\alpha_0(5d_{3/2})$ (88.5%) is from the three transitions $5d_{3/2}-6p_{1/2}$, $5d_{3/2}-6p_{3/2}$, and $5d_{3/2}-5f_{5/2}$. Similarly, the largest contribution to $\alpha_0(5d_{5/2})$ (86.3%) is from the three transitions $5d_{5/2}-6p_{3/2}$, $5d_{5/2}-5f_{5/2}$, and $5d_{5/2}-5f_{7/2}$ (see the fifth column in Table VI). Among these three contributions, the largest is from the $5d_{5/2}-6p_{3/2}$ transition.

Contributions to the tensor polarizabilities $\alpha_2(5d_{3/2})$ and $\alpha_2(5d_{5/2})$ are listed in columns 3 and 6 in Table VI. The $5d_{3/2}-6p_{1/2}$ transition contributes 102% of the “Total” shown on the

last line of Table VI since two other contributions ($5d_{3/2}-6p_{3/2}$ and $5d_{3/2}-5f_{5/2}$) partially cancel each other. A similar behavior is found for $\alpha_2(5d_{5/2})$. The $5d_{5/2}-6p_{3/2}$ transition contributes 87.6% of the “Total” shown in the last row in Table VI. An additional 10% contribution is from the $5d_{5/2}-5f_{5/2}$ transition. Contributions of transitions to highly excited states such as $(9-26)p_{1/2}$, $(9-26)p_{3/2}$, $(10-26)f_{5/2}$, and $(10-26)f_{7/2}$ are small.

Contributions to the scalar polarizabilities of $6p$ levels are listed in the second and fourth columns, respectively, in Table VII and contributions to the tensor polarizability $\alpha_2(6p_{3/2})$ are listed in column 5 in Table VII.

TABLE VII. Contributions to the scalar and tensor polarizabilities of the $6p_{1/2}$ and $6p_{3/2}$ states of Lu^{2+} , in a_0^3 . Uncertainties are given in e.

Contribution	$\alpha_0(6p_{1/2})$	Contribution	$\alpha_0(6p_{3/2})$	$\alpha_2(6p_{3/2})$
$6s_{1/2}$	-10.234(74)	$6s_{1/2}$	-8.747(70)	8.747(70)
$7s_{1/2}$	4.009(35)	$7s_{1/2}$	6.549(224)	-6.549(224)
$(8-26)s_{1/2}$	0.344(10)	$(8-26)s_{1/2}$	0.389(31)	-0.389(31)
		$5d_{3/2}$	-0.743(27)	-0.594(21)
		$6d_{3/2}$	2.180(29)	1.744(23)
		$7d_{3/2}$	0.069(1)	0.056(1)
		$8d_{3/2}$	0.013(0)	0.010(0)
		$(9-26)d_{3/2}$	0.021(0)	0.017(0)
$5d_{3/2}$	-9.585(318)	$5d_{5/2}$	-7.938(265)	1.588(53)
$6d_{3/2}$	15.382(286)	$6d_{5/2}$	18.638(171)	-3.728(34)
$7d_{3/2}$	0.716(5)	$7d_{5/2}$	0.668(6)	-0.134(1)
$8d_{3/2}$	0.154(0)	$8d_{5/2}$	0.131(0)	-0.026(0)
$9d_{3/2}$	0.055(0)	$9d_{5/2}$	0.046(0)	-0.009(0)
$(10-26)d_{3/2}$	0.181(0)	$(10-26)d_{5/2}$	0.096(0)	-0.019(0)
Core	4.264(080)	Core	4.264(080)	0.0
Term-vc	-0.001(0)	Term-vc	0.0(0)	0.0
Tail	0.0	Tail	0.0	0.0
Total	5.24(44)	Total	15.63(41)	0.71(25)

TABLE VIII. Dynamic correction to the BBR shift of the $6s-5d$ clock transition in Lu^{2+} at $T = 30$ K (in Hz).

	η	$\alpha_0(\omega = 0)$	$\Delta v_{\text{BBR}}^{\text{dyn}}$
$6s_{1/2}-6p_{1/2}$	0.000178		
$6s_{1/2}-6p_{3/2}$	0.000224		
Total ($6s_{1/2}$)	0.000402	31.91	-0.000110
$5d_{5/2}-6p_{3/2}$	0.000276		
$5d_{5/2}-5f_{5/2}$	0.0000006		
$5d_{5/2}-5f_{7/2}$	0.000012		
Total ($5d_{5/2}$)	0.000288	12.09	-0.000030
Final $\Delta v_{\text{BBR}}^{\text{dyn}}(5d_{5/2}-6s_{1/2})$			0.000080

V. BLACKBODY RADIATION SHIFT

Calculations of BBR shifts of clock frequencies in the monovalent ions Ca^+ and Sr^+ were presented in Refs. [29,38–40]. The BBR shift for the $4s_{1/2}-3d_{5/2}$ transition in $^{43}\text{Ca}^+$ was calculated by Arora *et al.* [38] using the all-order SD method. The SD method was also used by Jiang *et al.* [39] to calculate the BBR shift of the $5s_{1/2}-4d_{5/2}$ clock transition in $^{88}\text{Sr}^+$. A review of recent theoretical calculations of BBR shifts in optical atomic clocks was presented by Safronova *et al.* [40].

The amplitude of the frequency-dependent electric field E radiated by a black body at temperature T is given by the Planck radiation law [38]. The frequency shift of an ionic state v due to such an electric field is related to the static scalar polarizability $\alpha_0(v)$ of the state by

$$\Delta v = -\frac{1}{2}(831.9 \text{ V/m})^2 \left(\frac{T(\text{K})}{300}\right)^4 \alpha_0(v)(1 + \eta), \quad (3)$$

where η is a small “dynamic” correction [41,42]. We find that this dynamic correction is negligible compared to the present 3% uncertainty of our calculated scalar polarizabilities. The isotropic nature of the BBR field leads to the averaging-out of the tensor polarizability effects. The BBR shift of the clock

TABLE IX. Hyperfine constants A (in MHz) in $^{175}\text{Lu}^{2+}$ ($I = 7/2$, $\mu = 2.2327 \mu_N$ [43]). Theoretical SD and SDpT results are compared with MBPT results and experimental data [17].

Level	$A^{(\text{DF})}$	$A^{(\text{SD})}$	$A^{(\text{SDpT})}$	$A^{(\text{MBPT})}$	$A^{(\text{expt.})}$
$6s_{1/2}$	10311.3	13158.4	13176.8	13208.3	13070(60)
$7s_{1/2}$	3466.9	4135.6	4140.2	4137.3	4200(600)
$8s_{1/2}$	1610.3	1877.3	1879.3	1876.2	1860(300)
$9s_{1/2}$	880.2	1012.4	1015.1	1014.2	
$5d_{3/2}$	398.3	504.7	516.5	543.3	
$5d_{5/2}$	152.5	-10.2	-6.3	-11.3	
$6d_{3/2}$	87.0	111.7	110.9	114.8	
$6d_{5/2}$	34.1	24.2	24.5	25.0	
$7d_{3/2}$	38.9	50.4	49.8	50.5	
$7d_{5/2}$	15.4	13.8	13.8	13.6	
$6p_{1/2}$	2007.8	2778.3	2779.6	2799.7	2520(60)
$6p_{3/2}$	232.6	371.1	372.2	360.1	390(90)
$7p_{1/2}$	786.7	1015.3	1014.2	1027.3	
$7p_{3/2}$	93.1	186.3	186.2	137.9	
$8p_{1/2}$	391.9	477.8	477.2	500.0	
$8p_{3/2}$	46.9	136.0	149.1	68.6	

transition frequency is the difference between the BBR shifts of the states involved in the clock transition. The static BBR shift is

$$\begin{aligned} & \Delta(5d_{5/2} - 6s_{1/2}) \\ &= -\frac{1}{2} \left[\alpha_0(5d_{5/2} - 6s_{1/2})(831.9 \text{ V/m})^2 \left(\frac{T(\text{K})}{300}\right)^4 \right]. \quad (4) \end{aligned}$$

Evaluation of the BBR shift of the $5d_{5/2}-6s_{1/2}$ clock transition frequency in Lu^{2+} , therefore, involves accurate calculations of the static scalar polarizabilities of the $6s$ ground state and the $5d_{5/2}$ excited state. Here we use the scalar polarizabilities $\alpha_0(6s_{1/2}) = 31.91 \pm 0.18$, listed in Table V, and $\alpha_0(5d_{5/2}) = 12.09 \pm 0.20$, listed in Table VI. The resulting BBR shift of the clock transition in Lu^{2+} is

$$\Delta_{\text{BBR}}(5d_{5/2} - 6s_{1/2}) = 0.1706 \pm 0.0023 \text{ Hz.}$$

The $6s_{1/2}-5d_{5/2}$ transition frequency is $\nu_0(\text{Hz}) = 2.59 \times 10^{14}$ Hz and the ratio of the BBR shift to the transition frequency is 6.581×10^{-16} , with an uncertainty of 0.089×10^{-16} .

In Table VIII, we present results for the dynamic corrections to the BBR shift of the clock transition in Lu^{2+} at $T = 300$ K. As mentioned earlier, the final dynamic shift, $\Delta v_{\text{BBR}}^{\text{dyn}}(5d_{5/2}-6s_{1/2}) = 0.000080$ Hz, is so small that it can be neglected compared to the uncertainty induced by the polarizabilities (± 0.0023 Hz).

VI. HYPERFINE CONSTANTS FOR $^{175}\text{Lu}^{2+}$

Calculations of hyperfine constants follow the pattern described earlier for calculations of transition matrix elements. In Table IX, we list the hyperfine constants A for $^{175}\text{Lu}^{2+}$ and compare our values with available experimental measurements [17]. In this table, we list the lowest-order $A^{(\text{DF})}$ and all-order $A^{(\text{SD})}$ and $A^{(\text{SDpT})}$ values for the ns , np , and nd levels up to $n = 8$. The nuclear spin and nuclear magnetic dipole moment of $^{175}\text{Lu}^{2+}$ used in these calculations are

TABLE X. Hyperfine constants B (in MHz) in $^{175}\text{Lu}^{2+}$. The nuclear quadrupole moment of $^{175}\text{Lu}^{2+}$ is $Q = 3.396$ b [44]. Theoretical SD and SDpT results are compared with MBPT calculations.

Level	$B^{(\text{DF})}$	$B^{(\text{SD})}$	$B^{(\text{SDpT})}$	$B^{(\text{MBPT})}$
$5d_{3/2}$	1432.7	1957.4	2001.1	2040.6
$5d_{5/2}$	1692.4	2456.4	2509.8	2499.5
$6d_{3/2}$	312.9	541.6	540.2	547.7
$6d_{5/2}$	378.4	696.4	694.7	700.2
$7d_{3/2}$	140.1	239.7	238.1	241.0
$7d_{5/2}$	170.4	308.3	306.4	308.4
$6p_{3/2}$	2483.5	3803.5	3811.8	3813.4
$7p_{3/2}$	994.4	1427.0	1426.5	1436.3
$8p_{3/2}$	500.9	645.7	642.3	689.2

$I = 7/2$ and $\mu = 2.2327\mu_N$, respectively [43]. Differences between $A^{(\text{SD})}$ and $A^{(\text{SDpT})}$ are generally about 0.2%, while the ratios $A^{(\text{SD})}$ to $A^{(\text{DF})}$ are 1.3–2.0 for some cases. The largest difference between $A^{(\text{SD})}$ and $A^{(\text{SDpT})}$ (about a factor of 2) occurs for the $5d_{5/2}$ level. For this state, even the signs of $A^{(\text{DF})}$ and $A^{(\text{SD})}$ are different and the ratio of the magnitudes of $A^{(\text{DF})}$ and $A^{(\text{SD})}$ is equal to 15. The difference between $A^{(\text{SD})}$ and $A^{(\text{MBPT})}$ for the $5d_{5/2}$ state is smaller than that between $A^{(\text{SD})}$ and $A^{(\text{SDpT})}$, emphasizing the importance of higher-order correlation corrections for this transition.

We use the differences between $A^{(\text{SD})}$ and $A^{(\text{SDpT})}$ to estimate the uncertainty in our calculations. Taking into account the uncertainties in the experimental values [17], we conclude that our results agree with the experimental values, which are listed in the last column in Table IX. The largest difference between theory and experiment (9%) is for the $6p_{1/2}$ level, while the uncertainty given in Ref. [17] for the $6p_{1/2}$ level is about 2%.

Hyperfine constants B (in MHz) for $^{175}\text{Lu}^{2+}$ are listed in Table X. The nuclear quadrupole moment of ^{175}Lu is $Q = 3.396$ b [44]. Calculations of $B^{(\text{DF})}$, $B^{(\text{SD})}$, $B^{(\text{SDpT})}$, and

$B^{(\text{MBPT})}$ are listed in Table X. The differences between $B^{(\text{SD})}$ and $B^{(\text{SDpT})}$ are in the range 0.1%–0.5% for all cases except the $5d$ levels, where $B^{(\text{SD})}$ and $B^{(\text{SDpT})}$ differ by about 2%. The ratios of the $B^{(\text{SD})}$ and $B^{(\text{SDpT})}$ are in the range 1.4–2.0 for all levels listed in Table X, confirming the importance of the correlation in the present calculations. Values of $B^{(\text{MBPT})}$ and $B^{(\text{SDpT})}$ differ by about 2%.

VII. CONCLUSION

In summary, we have carried out a systematic high-precision study of the energies, transition matrix elements, polarizabilities, blackbody shifts, and hyperfine constants for the ns , np , nd , and nf ($n \leq 9$) states of Lu^{2+} using a relativistic all-order approach. Recommended values of the atomic parameters are given along with estimates of the corresponding uncertainties. The theoretical energy values are in excellent agreement with existing experimental data. Recommended values together with uncertainties are provided for a large number of electric-dipole matrix elements. Scalar and tensor polarizabilities are evaluated for the ground state and low-lying excited states in Lu^{2+} . The BBR shift of the $6s_{1/2}$ – $5d_{5/2}$ clock transition frequency in Lu^{2+} [$\Delta_{\text{BBR}}(6s_{1/2}$ – $5d_{5/2})$] is found to be 0.1706 ± 0.0023 Hz $^{175}\text{Lu}^{2+}$. Finally, the hyperfine constants A and B of $^{175}\text{Lu}^{2+}$ are determined for low-lying levels up to $n = 9$. This work has provided recommended values of atomic properties of the ion Lu^{2+} , critically evaluated for accuracy, in a systematic high-precision study. These values may be useful for benchmark tests of theory, astrophysics applications, and planning and analysis of various experiments that depend on the level structure of the ion Lu^{2+} , including atomic clocks.

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