Relativistic all-order many-body calculation of energies, wavelengths, and $M1$ and $E2$ transition rates for the $3d^n$ configurations in tungsten ions

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Energy levels, wavelengths, magnetic-dipole and electric-quadrupole transition rates between the low-lying states are evaluated for W^{51+} to W^{54+} ions with $3d^n$ ($n = 2$ to 5) electronic configurations by using an approach combining configuration interaction with the linearized coupled-cluster single-double method. The QED corrections are directly incorporated into the calculations and their effect is studied in detail. Uncertainties of the calculations are discussed. This study of such highly charged ions with the present method opens the way for future applications allowing an accurate prediction of properties for a very wide range of highly charged ions aimed at providing precision benchmarks for various applications.

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I. INTRODUCTION

Theoretical and experimental studies of tungsten highly charged ions with an open $3d$ shell is at present a subject of extensive research [1–4] motivated, in part, by the proposed use of tungsten as a plasma-facing material in the divertor region of the international reactor ITER [5]. The core temperatures on the order of 10–20 keV are not sufficient to completely ionize tungsten, and its partially ionized atoms are expected to strongly emit in the x-ray and extreme ultraviolet (EUV) ranges of spectra. The measured radiation can be reliably used to diagnose certain plasma properties such as temperature and density. This application stimulated an extensive analysis of the EUV spectra between 10 and 25 nm from highly charged ions of tungsten with an open $3d$ shell [1] carried out at NIST. By using an electron-beam ion trap (EBIT), a number of forbidden magnetic-dipole lines within ground configurations of all $3d^n$ ions of tungsten, from Co-like W^{47+} to K-like W^{55+} were measured and identified in the spectra [1]. This work demonstrated that almost all strong lines were due to the forbidden magnetic-dipole ($M1$) transitions within $3d^n$ ground configurations. Further study of extreme-ultraviolet $M1$ lines in 50-60-fold ionized atoms of tungsten, hafnium, tantalum, and gold with an open $3d$ shell was reported in Ref. [6]. Using EBIT the spectra were measured at NIST and large-scale collisional-radiative modeling was instrumental in line identification and in analysis of their diagnostic potential. Furthermore, the $M1$ line ratios were shown to be an accurate and versatile tool for studying the dielectronic resonances in $3d^n$ ions including effects of anisotropy of the EBIT electron energy distribution function [7].

Motivated by such interest in the $M1$ transitions in open-shell highly charged ions (HCIs) with $3d^n$ configuration, we carry out a high-precision benchmark study of tungsten HCIs by using the state-of-the-art method which combines configuration interaction (CI) with the linearized coupled-cluster method, refereed to as the CI + all-order method [8]. The CI + all-order method was used to accurately evaluate properties of atomic systems with two to four valence electrons [9–16], including superheavy elements No, Lr, and Rf [17]. An advantage of this approach is the ability to include core correlations for all core shells together with the accurate description of the valence electronic correlations. The method was recently applied to low and medium ionization charge HCIs, up to 17^+ [15,18–20], to predict their properties relevant to the new proposals to use HCIs for the development of ultraprecise frequency standards and a search for variation of the fine-structure constant [21]. In 2016, the QED corrections were incorporated directly into the CI + all-order method by Tupitsyn *et al.* [22]. The authors compared the performance of four different QED potentials to estimate the accuracy of QED calculations and made a prediction of HCI properties urgently needed for planning future experiments of interest to metrology and tests of fundamental physics [22].

In this work, we use a new version of the CI + all-order + QED method developed in Ref. [22] to study the properties of HCIs with much higher degree of ionization, up to W^{54+}. We also conducted a detailed study of the QED corrections, carrying out all of the calculations with and without inclusion of the QED to demonstrate the size of the QED contribution. This effort paves the way for future applications of this approach for an accurate prediction of properties for a very

wide range of HCIs and providing precision benchmarks for spectra identification and other applications. This is also the first calculation of the system with five valence electrons with the CI + all-order method.

We start with a summary of previous relevant theoretical studies. Energy levels of the $3d^k$, $k = 1$–9, configurations for tungsten ions, computed by using the fully relativistic multiconfiguration Dirac–Hartree–Fock (MCDHF) GRASP2K code [23], based on the variational method, were reported by Froese Fisher *et al.* [4]. The correlation corrections for the $3s$, $3p$, and $3d$ orbitals considered to be valence orbitals, as well as the core-core and core-valence effects from the $2s$ and $2p$ subshells, were included in the calculations. Extensive MCDHF calculations were also performed for the $3s^2 3p^6 3d^k$ ($k = 1$–9) ground configurations of HCIs with $Z = 72$–83 in Ref. [3]. Complete and consistent data sets of excitation energies, wavelengths, line strengths, oscillator strengths, and magnetic-dipole and electric-quadrupole ($E2$) transition rates among all these levels were given and compared with the results available in the literature.

The wavelengths and transition probabilities are computed in Ref. [24] for forbidden transitions within the $3d^k$ ($k = 1$–9) ground configurations in ions of hafnium, tantalum, tungsten, and gold. The authors used the second-order relativistic many-body perturbation theory (RMBPT) following the method described in Ref. [25].

The excitation energies and transition rates for the states within the $3d^2$ configuration of Ca-like ions with $Z = 22$–100 were calculated by Safronova *et al.* in Ref. [28]. The method based on RMBPT, including the Breit interaction, was used to evaluate the matrix elements of $M1$ and $E2$ operators, including the retardation and contribution from negative–energy states. The wavelengths and $M1$ and $E2$ transition rates for Ca-like tungsten were reported in Ref. [27]. The results were obtained in the framework of the RMBPT. The first-order perturbation theory was used to obtain intermediate coupling coefficients and the second-order RMBPT was used to determine the matrix elements.

The wavelengths and transition rates were computed by Quinet [29] for forbidden transitions within the $3d^k$ ground configurations of tungsten ions from W^{47+} to W^{61+} using a fully relativistic multiconfiguration Dirac–Fock method. The single and double excitations within the $n = 3$ complex, some $n = 3 \rightarrow n' = 4$ single excitations, the Breit interaction, and the QED effects were included.

The atomic structure and spectra of ten tungsten ions were calculated by using the Flexible Atomic Code (FAC) by Clementson *et al.* [30]. The energy levels, radiative lifetimes, spectral line positions, transition probability rates, and oscillator strengths for the tungsten ions isoelectronic to germanium, W^{42+}, through vanadium, W^{51+}, were reported.

II. CONFIGURATION INTERACTION + ALL-ORDER METHOD

For evaluation of the atomic properties of Ca-like, Sc-like, Ti-like, and V-like W ions we use the CI + all-order method which is based on a combination of configuration interaction with a linearized coupled-cluster single-double method [8]. The energies, wavelengths, and transition rates of the low-lying levels are evaluated. The wavelengths obtained in the framework of this approach are compared with the experimental energies [1] where available.

In the CI + all-order approach, the one- and two-electron corrections to the effective Hamiltonian, Σ_1 and Σ_2, are calculated by using a modified version of the linearized coupled-cluster (all-order) method with single and double excitations described in Ref. [31,32]. As a result, the effective Hamiltonian contains dominant core-valence and core-core correlation corrections to all orders. A most complicated and time-consuming problem is to efficiently calculate the all-order correction $\Sigma_2(ijkl)$. We carry out calculations as follows:

(1) The single-double all-order calculations are carried out for Ar-like core, including seven relativistic subshells, starting with $1s$. Single and double excitations are allowed from *all* core subshells. This includes core-core correlations.

(2) Using the all-order results for the core orbitals, the single-double core-valence all-order calculations are carried out for 24 valence orbitals: $4s$–$7s$, $4p_{1/2}$–$7p_{1/2}$, $4p_{3/2}$–$7p_{3/2}$, $3d_{3/2}$–$6d_{3/2}$, $3d_{5/2}$–$6d_{5/2}$, $4f_{5/2}$–$5f_{5/2}$, and $4f_{7/2}$–$5f_{7/2}$. The core excitations are also allowed from *all* core subshells. The all-order method is modified to exclude valence diagrams that will be later accounted for by the CI. This part of the calculation produces the Σ_1 and $\Sigma_2(ijva)$ quantities, where i and j can be any excited state, a is the core state, and v are the 24 orbitals from the list given above.

(3) The $\Sigma_2(ijvw)$ corrections to the CI Hamiltonian are calculated, with w also taken from the above valence list. We tested that restricting the all-order calculation to 24 valence orbitals results in sufficient numerical accuracy. We note that the remaining $\Sigma_2(ijkl)$ elements are still corrected in the second order of MBPT. More details of the CI + all-order approach are given in Ref. [8]. All of the second- and all-order calculations include partial waves with the orbital quantum numbers $l = 0$-6.

(4) The CI method [33] is then used to treat valence-valence correlations, with the CI code modified to include effective Hamiltonian constructed as described above. The CI space (constructed as described, e.g., in Ref. [34]) includes configurations with 2–5 valence electrons, depending on the considered ion.

The QED correction is incorporated into the basis set orbital via the model QED potentials described in detail in Ref. [22]. The QED corrections are added to the one-electron matrix elements of the effective Hamiltonian, which is constructed as described above and includes the Dirac–Fock–Breit potential of the core and the Coulomb–Breit interactions of the valence electrons [8].

III. CALCIUM-LIKE W^{54+} ION

The CI + all-order method was used to evaluate the Ca-like W^{54+} ion energies, wavelengths, and $M1$ and $E2$ transition rates between the states within the $3d^2$ configuration. In Table I, we present the energies of the low-lying states and compare them with the recommended NIST data [26] and theoretical results obtained by using RMBPT from Ref. [27] and the MCDHF method [4] implemented by using the GRASP2K code.

To identify the terms (assuming that LS coupling is approximately valid), we calculated the g factors of the states

TABLE I. Ca-like W^{54+}. The low-lying energy levels (in cm^{-1}) calculated by using the CI + all-order method are given in columns BREIT and QED. They are compared with the recommended NIST data [26], labeled NIST, and theoretical results from Refs. [27] and [4], labeled RMBPT and GRASP2K, respectively. The first row gives the absolute value of the ground-state valence energy. The energies of the excited states are counted from the ground-state energy. The columns labeled BREIT and QED list the results which include the Breit interaction obtained without and with the QED corrections, respectively. The differences between the NIST and RMBPT, NIST and BREIT, and NIST and QED values are shown in % and cm^{-1} in columns labeled N − R, N − B, and N − Q, respectively.

						Difference in %			Difference in cm^{-1}		
Level	NIST [26]	RMBPT [27]	GRASP2K [4]	BREIT	QED	N − R	N − B	N − Q	N − R	N − B	N − Q
$3d^2\ ^3F_2$	85150000			85045940	85053834		0.12	0.11		104060	96166
$3d^2\ ^3P_0$	188000	187110	186230	186228	186100	0.47	0.94	1.01	890	1772	1900
$3d^2\ ^3F_3$	585480	582850	584750	584212	585659	0.45	0.22	−0.06	2630	1268	−379
$3d^2\ ^3D_2$	668490	666210	667960	667321	668700	0.34	0.17	−0.03	2280	1169	−210
$3d^2\ ^3G_4$	697000	693810	696100	695931	697355	0.46	0.15	−0.05	3190	1069	−355
$3d^2\ ^3P_1$	709460	705410	706750	706048	707428	0.57	0.48	0.29	4050	3412	2032
$3d^2\ ^3F_4$	1234000	1231640	1235570	1234504	1237339	0.19	−0.04	−0.27	2360	−504	−3339
$3d^2\ ^1D_2$	1299000	1296730	1300180	1298669	1301477	0.17	0.03	−0.19	2270	331	−2477
$3d^2\ ^1S_0$	1493000	1491540	1493710	1492483	1495148	0.10	0.03	−0.14	1460	517	−2148

and compared them with the nonrelativistic values g_{nr}, given by the Landé formula,

$$g_{nr} = \frac{3}{2} + \frac{S(S+1) - L(L+1)}{2J(J+1)}. \quad (1)$$

Based on this comparison and knowing the total angular momenta J of levels, we assigned the spin S and orbital L quantum numbers to the terms, listed in Table I. We note that jj coupling is frequently used to label states of HCI ions with a high degree of ionization.

The first line of the table gives the two-electron binding energy of the ground state of this divalent ion, found as the sum of two ionization potentials (IPs): $IP(W^{54+}) + IP(W^{55+})$. The energies of other states are counted from the ground-state energy. In the columns labeled BREIT and QED, the results, obtained in the framework of the CI + all-order approach, are presented. Both include the Breit interaction, but the QED results additionally include the QED corrections. The results listed in the QED column are the final values.

The differences between NIST and RMBPT, NIST and BREIT, and NIST and QED values are shown in percent and cm^{-1} in columns labeled N − R, N − B, and N − Q, respectively. Except for the result for the $^3P_0$ state, the values in the N − B column are substantially smaller than the values

TABLE II. Wavelengths (in nm) and A_{M1} and A_{E2} transition rates (in s^{-1}) in W^{54+} are compared with the available theoretical [27] and experimental [1] results. Numbers in brackets represent powers of 10.

Transition		λ, nm			A_{M1}		A_{E2}	
Final	Initial	Present	Ref. [27]	Ref. [1]	Present	Ref. [27]	Present	Ref. [27]
$^3F_2$	$^1D_2$	7.700	7.712		1.14[4]	1.276[4]	1.26[1]	4.507[1]
$^3F_2$	$^3F_4$	8.100	8.119				2.21[2]	4.304[2]
$^3P_1$	$^1S_0$	12.716	12.721		7.79[6]	7.323[6]		
$^3F_3$	$^1D_2$	13.997	14.008		7.48[5]	7.524[5]	1.06[3]	1.052[3]
$^3F_2$	$^3P_1$	14.163	14.176		2.60[5]	2.583[5]	9.67[2]	1.179[3]
$^3F_2$	$^3G_4$	14.369	14.413				4.22[2]	3.219[2]
$^3F_2$	$^3D_2$	14.985	15.010	14.959	1.79[6]	1.798[6]	7.74[2]	7.312[2]
$^3F_3$	$^3F_4$	15.378	15.413		3.79[6]	3.755[6]	7.19[1]	6.133[1]
$^3D_2$	$^1D_2$	15.839	15.860		3.08[6]	3.095[6]	1.00[2]	7.536[1]
$^3G_4$	$^1D_2$	16.591	16.586				1.41[0]	1.998[1]
$^3P_1$	$^1D_2$	16.874	16.911		1.29[6]	1.285[6]	3.56[2]	4.184[2]
$^3F_2$	$^3F_3$	17.117	17.157	17.080	3.66[6]	3.683[6]	1.23[2]	1.154[2]
$^3D_2$	$^3F_4$	17.631	17.686				1.84[2]	6.397[1]
$^3G_4$	$^3F_4$	18.568	18.593		1.09[6]	1.110[6]	3.51[2]	7.548[2]
$^3P_0$	$^3P_1$	19.237	19.294	19.177	1.72[6]	1.771[6]		
$^3F_3$	$^3P_1$	82.078	81.595				8.20[−1]	9.071[−1]
$^3F_3$	$^3G_4$	89.510	90.123		8.41[3]	8.556[3]	2.70[−3]	4.237[−5]
$^3F_3$	$^3D_2$	120.325	119.974		4.32[3]	4.351[3]	1.14[−2]	2.145[−2]
$^3F_4$	$^1D_2$	155.851	153.641				2.78[−2]	3.740[−3]
$^3D_2$	$^3P_1$	258.211	253.066		6.40[2]	6.788[2]	2.88[−3]	3.731[−3]
$^3D_2$	$^3G_4$	349.516	362.222				1.90[−4]	8.126[−4]

in the N − R column. It demonstrates that our CI + all-order method gives more accurate results than the second-order RMBPT, and that the higher orders are important even for such highly charge ions. Comparing the NIST and all-order results for the valence energy of the ground state, we see an excellent agreement.

The QED corrections to the ground state and transition energies are small, not exceeding 0.3%, but significant for the precision calculation for Ca-like W^{54+}, as seen from a comparison of the results in the N − B and N − Q columns.

We also evaluated the probabilities of $M1$ and $E2$ transitions between the states listed in Table I. For a transition from the $|J\rangle$ to $|J'\rangle$ state, the $M1$ and $E2$ transition rates A_{M1} and A_{E2}, in s^{-1}, are expressed through reduced matrix elements and the transition wavelength λ (in nm) as follows:

$$A_{M1} = \frac{2.69735 \times 10^{10}}{\lambda^3(2J+1)}|\langle J'||\mu||J\rangle|^2,$$
$$A_{E2} = \frac{1.11995 \times 10^{13}}{\lambda^5(2J+1)}|\langle J'||Q||J\rangle|^2. \quad (2)$$

Here μ and Q are the magnetic-dipole and electric-quadrupole operators. The reduced matrix elements of μ and Q are given in Bohr magnetons and atomic units (ea_0^2, where a_0 is the Bohr radius), respectively.

In Table II we list the wavelengths and $M1$ and $E2$ transition rates for 21 transitions evaluated using the CI + all-order method, including the Breit interaction. Our values of the wavelengths are compared with the results obtained using RMBPT in Ref. [27]. We observe a very small (0.1%–0.3%) difference in wavelengths obtained in this work and in Ref. [27] for a majority of transitions. The largest difference is observed for the $^3F_3$-$^3P_1$, $^3F_3$-$^3P_2$, $^3F_4$-$^1D_2$, $^3P_2$-$^3P_1$, and $^3P_2$-$^3G_4$ transitions. There are three experimentally known wavelengths, measured by Ralchenko *et al.* [1]. A comparison of our results with the experiment (see Table II) shows an excellent agreement (0.17%, 0.22%, and 0.31%) between them. Other wavelengths are compared with experiment in Table III.

The values of A_{M1} obtained in this work and in Ref. [27] and given by columns 6 and 7 in Table II are in a reasonable agreement. The maximum difference is ∼10%. The difference in $E2$ transition rates, listed in two last columns of Table II, is substantially larger, especially for the transitions with small (10^{-5}–10^{-3} s^{-1}) rates.

The probability of the $M1$ transition is typically a few orders of magnitude larger than the probability of the $E2$ transition for the transitions consider here, which involve no change in the principal quantum number because all states are within the same configuration since the $3d^2$ configuration gives an absolutely dominating (∼99.9% in probability) contribution to all states listed in Tables I and II. For this reason a mixture of configurations practically does not influence the magnitude of the matrix elements. The matrix elements (MEs) of the electric-quadrupole operator ($Q \sim r^2$) are determined by the behavior of the wave functions at large distances. For such a highly charged ion as W^{54+}, the $3d_{3/2,5/2}$ valence orbitals are very rigid; their root-mean-square radius is ∼0.2 a.u. It leads to a smallness of $\langle J'||Q||J\rangle$.

TABLE III. Wavelengths (nm) for transitions within the $3d^2$ configuration in Ca-like W^{54+} evaluated using the CI + all-order method without and with QED contributions. The wavelengths are compared with available measurements from Ref. [1].

Transition		Wavelengths, λ, nm		
		No QED	QED	Expt. [1]
$3d^2\ ^3F_2$	$3d^2\ ^1S_0$	6.700	6.688	
$3d^2\ ^3F_2$	$3d^2\ ^1D_2$	7.699	7.684	
$3d^2\ ^3F_2$	$3d^2\ ^3F_4$	8.099	8.082	
$3d^2\ ^3P_0$	$3d^2\ ^1D_2$	8.987	8.966	
$3d^2\ ^3P_2$	$3d^2\ ^1S_0$	12.119	12.100	
$3d^2\ ^3P_1$	$3d^2\ ^1S_0$	12.716	12.695	
$3d^2\ ^3F_3$	$3d^2\ ^1D_2$	13.996	13.970	
$3d^2\ ^3F_2$	$3d^2\ ^3P_1$	14.162	14.136	
$3d^2\ ^3F_2$	$3d^2\ ^1G_4$	14.368	14.340	
$3d^2\ ^3F_2$	$3d^2\ ^3P_2$	14.984	14.954	14.959
$3d^2\ ^3F_3$	$3d^2\ ^3F_4$	15.376	15.345	
$3d^2\ ^3P_2$	$3d^2\ ^1D_2$	15.837	15.803	
$3d^2\ ^1G_4$	$3d^2\ ^1D_2$	16.588	16.553	
$3d^2\ ^3P_1$	$3d^2\ ^1D_2$	16.871	16.834	
$3d^2\ ^3F_2$	$3d^2\ ^3F_3$	17.113	17.075	17.080
$3d^2\ ^3P_2$	$3d^2\ ^3F_4$	17.627	17.586	
$3d^2\ ^1G_4$	$3d^2\ ^3F_4$	18.563	18.519	
$3d^2\ ^3P_0$	$3d^2\ ^3P_1$	19.230	19.182	19.177
$3d^2\ ^3P_0$	$3d^2\ ^3P_2$	20.777	20.721	
$3d^2\ ^1D_2$	$3d^2\ ^1S_0$	51.625	51.634	
$3d^2\ ^3F_2$	$3d^2\ ^3P_0$	53.740	53.735	
$3d^2\ ^3F_3$	$3d^2\ ^3P_1$	82.116	82.123	
$3d^2\ ^3F_3$	$3d^2\ ^1G_4$	89.544	89.529	
$3d^2\ ^3F_3$	$3d^2\ ^3P_2$	120.402	120.422	
$3d^2\ ^3F_4$	$3d^2\ ^1D_2$	155.926	155.914	
$3d^2\ ^3P_2$	$3d^2\ ^3P_1$	258.238	258.211	
$3d^2\ ^3P_2$	$3d^2\ ^1G_4$	349.382	348.979	

IV. SCANDIUM-LIKE W^{53+} ION

The energies, wavelengths, and transition rates of the $M1$ and $E2$ transitions between the states within the $3d^3$ configuration of the trivalent Sc-like W^{53+} ion are calculated. In Table IV, we list the low-lying energy levels for Sc-like W^{53+} evaluated in the BREIT and QED approximations. As we already mentioned above, the latter includes the QED corrections. We compare our results with the recommended NIST data [26] and theoretical results obtained in Ref. [24] using the revised version of the FAC code and MCDHF [4].

The first ionization potential is given in the first row. We find it as the difference between the ground-state valence energy of Sc-like W^{53+} and the ground-state valence energy of Ca-like W^{54+} (given in the first row of Table I). The energies of other states are counted from the ground-state energy.

The designations used in the table are similar to those used previously for Ca-like W^{54+} ions. The differences between FAC and NIST, BREIT and NIST, and QED and NIST values are presented in the three last columns and labeled F − N, B − N, and Q − N, respectively. All four FAC, GRASP2K, BREIT, and QED results are in a good agreement with the experimental results and with each other. For a majority of energy levels the

TABLE IV. The calculated energy levels of Sc-like W^{53+} ion (in cm^{-1}) within the $3d^3$ configuration are listed in the columns BREIT and QED. They are compared with the recommended NIST data [26] and theoretical results from Refs. [4,24]. The first row gives the first ionization potential. The excited-state energies are counted from the ground-state energy. The differences (in%) between FAC and NIST, BREIT and NIST, and QED and NIST values are presented by the three last columns and labeled F − N, B − N, and Q − N, respectively. The g factors given by the Landé formula (nr) and calculated by the CI + all-order method (BREIT) are presented in columns 7 and 8.

	Energies					g factor		Difference (in %)		
Level	NIST [26]	FAC [24]	GRASP2K [4]	BREIT	QED	nr	BREIT	F − N	B − N	Q − N
$^2D^1_{3/2}$	40833000			40770300	40774500	0.8000	0.7211		−0.15	−0.14
$^4F^1_{5/2}$	530030	530511	529070	528021	529544	1.0286	1.0512	0.09	−0.38	−0.09
$^4D^1_{3/2}$	580860	580864	579990	578123	579594	1.2000	1.1659	0.00	−0.47	−0.22
$^4H_{9/2}$	610000	611618	610860	610047	611577	0.9697	1.0321	0.26	0.01	0.26
$^4G_{7/2}$	610000	611860	610320	610264	611802	0.9841	1.0355	0.30	0.04	0.29
$^2D^1_{5/2}$	812200	812220	812070	811936	813338	1.2000	1.2363	0.00	−0.03	0.14
$^2F^1_{7/2}$	1125950	1126000	1128600	1126911	1129889	1.1429	1.1156	0.00	0.09	0.35
$^2G_{9/2}$	1163858	1164000	1165990	1164377	1167384	1.1111	1.1285	0.01	0.04	0.30
$^4D^2_{3/2}$	1205798	1206000	1207730	1206422	1209376	1.2000	1.1057	0.02	0.05	0.30
$^2H_{11/2}$	1243513	1243000	1243300	1242189	1245195	1.0909	1.0791	−0.04	−0.11	0.14
$^2D^2_{5/2}$	1243706	1244000	1244610	1243569	1246465	1.2000	1.2878	0.02	−0.01	0.22
$^4F^2_{5/2}$	1314683	1315000	1315540	1314506	1317477	1.0286	1.0911	0.02	−0.01	0.21
$^2F^2_{7/2}$	1320329	1320000	1319550	1318007	1320942	1.1429	1.0836	−0.02	−0.18	0.05
$^2D^2_{3/2}$	1481640	1482000	1481260	1480471	1483413	0.8000	0.8856	0.02	−0.08	0.12
$^4G_{9/2}$		1767023	1764860	1762772	1767221	1.1717	1.1576			
$^4D^3_{3/2}$		1878537	1878320	1875314	1879683	1.2000	1.1292			
$^2D^3_{5/2}$		1959564	1960120	1958695	1963041	1.2000	1.1607			

difference between the theory and experiment is only a few hundredth percent.

The g factors were also evaluated. Based on a comparison of the calculated values with the nonrelativistic values, given by the Landé formula, Eq. (1), we have identified terms in the LS coupling and made assignment of the quantum numbers. To distinguish between the terms which have the same S, L, and J quantum numbers in the LS coupling, we added an additional superscript on the right of the term designation.

In Table V, we list the wavelengths of selected transitions. Our results are in a good agreement with the four wavelengths measured in Ref. [1]. For the transitions in the region 10.5—19.9 nm we also calculated the $M1$ transition rates for the states within the $3d^3$ configuration in the BREIT and QED approximations. These results are listed in columns 6 and 7 of the table. There is a very good agreement between our values and the results of Ref. [1].

We observe that the QED corrections change the $M1$ transition rates only slightly. Typically, the difference between the BREIT and QED values is less than 1%. We do not list $E2$ transition rates because they are few orders of magnitude smaller than the $M1$ transition rates. The reason for this is the same as for the Ca-like W^{54+} ion.

V. TITANIUM-LIKE W^{52+} ION

In Table VI we list the low-lying energy levels for the tetravalent Ti-like W^{52+} ion calculated in the framework of the CI + all-order method not including the QED corrections (the BREIT approximation) and with the inclusion of QED. The recommended NIST data [26] and theoretical results of Refs. [4,24] are also given in the table. The QED corrections change the energies at the level of a few tenths of a percent. The first line gives the first ionization potential, with good agreement (0.16%) with the experiment. The energies of the excited states are counted from the ground-state energy. The

TABLE V. Sc-like W^{53+}. Wavelengths (in nm) and $M1$ transition rates (in s^{-1}) for the states within the $3d^3$ configuration are compared with the NIST data [1] where available. Numbers in brackets represent powers of 10.

Transition		Wavelength (nm)			$M1$ transition rate		
Final	Initial	BREIT	QED	Ref. [1]	BREIT	QED	Ref. [1]
$^4F^1_{5/2}$	$^4D^2_{3/2}$	10.499	10.484		6.73[5]	6.75[5]	
$^4D^1_{3/2}$	$^4D^2_{3/2}$	11.082	11.064		3.55[5]	3.55[5]	
$^2D^1_{3/2}$	$^2D^1_{5/2}$	12.316	12.294	12.312	2.78[5]	2.80[5]	2.75[5]
$^4F^1_{5/2}$	$^2F^2_{7/2}$	12.658	12.636		1.60[5]	1.60[5]	
$^4F^1_{5/2}$	$^2D^2_{5/2}$	13.975	13.949		4.32[5]	4.35[5]	
$^4H_{9/2}$	$^2F^2_{7/2}$	14.125	14.097		6.66[5]	6.70[5]	
$^4G_{7/2}$	$^2F^2_{7/2}$	14.129	14.102		7.51[5]	7.56[5]	
$^4G_{7/2}$	$^4F^2_{5/2}$	14.200	14.171		1.11[6]	1.12[6]	
$^4F^1_{5/2}$	$^4D^2_{3/2}$	14.741	14.710		1.97[6]	1.98[6]	
$^2D^1_{5/2}$	$^4D^2_{3/2}$	14.958	14.925		2.38[6]	2.40[6]	
$^4D^1_{3/2}$	$^2D^2_{5/2}$	15.028	14.995		2.48[6]	2.50[6]	
$^4G_{7/2}$	$^2D^2_{5/2}$	15.790	15.756		2.02[5]	2.02[5]	
$^4H_{9/2}$	$^2H_{11/2}$	15.819	15.782	15.785	1.42[6]	1.43[6]	1.42[6]
$^4F^1_{5/2}$	$^2F^1_{7/2}$	16.698	16.657		4.90[6]	4.94[6]	
$^2D^1_{3/2}$	$^4D^1_{3/2}$	17.297	17.253	17.216	2.75[6]	2.78[6]	2.74[6]
$^4H_{9/2}$	$^2G_{9/2}$	18.040	17.992		2.29[6]	2.30[6]	
$^4G_{7/2}$	$^2G_{9/2}$	18.047	17.999		1.30[6]	1.31[6]	
$^2D^1_{3/2}$	$^4F^1_{5/2}$	18.939	18.884	18.867	3.42[6]	3.42[6]	3.41[6]
$^4G_{7/2}$	$^2F^1_{7/2}$	19.356	19.302		1.19[6]	1.20[6]	
$^2D^1_{5/2}$	$^2F^2_{7/2}$	19.760	19.702		2.54[5]	2.56[5]	
$^2D^1_{5/2}$	$^4F^2_{5/2}$	19.898	19.838		1.13[6]	1.14[6]	

TABLE VI. Ti-like W^{52+} ion. The energies (in cm^{-1}) obtained in this work are listed in the columns BREIT and QED. They are compared with the recommended NIST data [26] and theoretical results [4,24]. First row gives the first ionization potential. The energies of the excited states are counted from the ground-state energy. The nonrelativistic g factor (nr) and g factor obtained using the CI + all-order method (BREIT) are presented.

	Energy (cm^{-1})					g factor	
Level	NIST [26]	FAC [24]	GRASP2K [4]	BREIT	QED	nr	BREIT
$3d^4\ ^3P_0^1$	39739000			39675100	39679450		
$3d^4\ ^3P_1$	517630	518082	516510	514599	516181	1.5000	1.4884
$3d^4\ ^3G_4^1$	613000	614788	613540	613414	615007	1.0500	1.0604
$3d^4\ ^3D_2^1$	638000	639339	638390	636589	638203	1.1667	1.1954
$3d^4\ ^3F_3^1$	665562	667036	666090	665288	666894	1.0833	1.1132
$3d^4\ ^5D_0$	1100000	1104665	1103180	1101522	1104648		
$3d^4\ ^3D_2^2$	1109690	1110020	1107980	1104742	1107800	1.1667	1.2765
$3d^4\ ^5G_4^1$	1127270	1129111	1126590	1124398	1127552	1.1500	1.1387
$3d^4\ ^5F_3^1$	1141000	1145194	1143020	1140618	1143757	1.2500	1.1752
$3d^4\ ^3H_5$	1173350	1175601	1173060	1171480	1174638	1.0333	1.0775
$3d^4\ ^5I_6^1$	1195000	1199023	1196310	1195327	1198507	1.0714	1.0663
$3d^4\ ^1P_1^1$	1213000	1215638	1214540	1211691	1214819	1.0000	1.0691
$3d^4\ ^3F_3^2$	1240000	1240988	1239920	1238038	1241125	1.0833	1.0606
$3d^4\ ^3G_4^2$	1243000	1244473	1243140	1242410	1245550	1.0500	1.0269
$3d^4\ ^1D_2^1$	1259000	1259426	1258620	1255734	1258834	1.0000	1.0777
$3d^4\ ^5F_2$	1361000	1360350	1360440	1358628	1361700	1.0000	0.9664
$3d^4\ ^5G_4^2$	1403000	1405106	1404220	1402530	1405591	1.1500	1.1774
$3d^4\ ^3D_2^3$	1509000	1505820	1506350	1504684	1507758	1.1667	1.1230
$3d^4\ ^1S_0^1$	1637000	1632740	1634150	1632102	1635268		
$3d^4\ ^5G_4^3$		1718501	1715100	1713475	1718101	1.1500	1.1620
$3d^4\ ^5F_3^3$		1729147	1727040	1724081	1728693	1.2500	1.1920
$3d^4\ ^1P_1^2$		1769701	1768580	1765900	1770496	1.0000	1.0001
$3d^4\ ^5H_5$		1777839	1775280	1772951	1777619	1.1000	1.1326
$3d^4\ ^5I_6^2$		1783283	1780210	1778186	1782877	1.0714	1.0771
$3d^4\ ^1D_2^2$		1843896	1842980	1838978	1843576	1.0000	1.0561
$3d^4\ ^3F_3^3$		1860180	1859240	1856826	1861430	1.0833	1.0858
$3d^4\ ^1S_0^2$		1923365	1924060	1924590	1929061		
$3d^4\ ^3F_3^5$		1981913	1981500	1978832	1983434	1.0833	1.0535
$3d^4\ ^5D_1$		1985438	1985440	1982097	1986656	1.5000	1.3963
$3d^4\ ^3G_4^3$		1987019	1986570	1984359	1988946	1.0500	1.0451
$3d^4\ ^3D_2^5$		2019676	2020040	2017244	2021769	1.1667	1.1083
$3d^4\ ^5G_4^5$		2380512	2378860	2376012	2382140	1.1500	1.1582
$3d^4\ ^3D_2^5$		2463555	2463080	2458818	2464864	1.1667	1.1038
$3d^4\ ^3P_0^2$		2663597	2665520	2663164	2669093		
$3d^3 4s\ ^3D_1$					15769907		
$3d^3 4s\ ^1D_2$					15782183		
$3d^3 4s\ ^1P_1$					16356332		
$3d^3 4s\ ^5F_2$					16305822		
$3d^3 4s\ ^3P_1$					16397221		

difference between the experiment and theory results is at the level of few tenths of a percent.

We have also calculated the g factors in the framework of the BREIT approximation and using the nonrelativistic formula (nr). By comparing these values we identified the terms listed in the table.

We calculated the magnetic-dipole transitions rates for 25 transitions in the region 12.8–20.9 nm. For the reasons discussed above the electric-quadrupole transition rates are a few orders of magnitude smaller and we disregard them. In Table VII we list the transition wavelengths (and compare them with the NIST data, where available) and the magnetic-dipole transitions rates. For the experimentally known wavelengths we find an excellent agreement with our calculated values.

VI. VANADIUM-LIKE W^{51+} ION

In Tables VIII and IX, we list the energies, wavelengths, and M1 transition rates for V-like W^{51+} calculated as a pentavalent ion in the framework of the CI + all-order method. For a comparison with the recommended NIST data [26] and theoretical results from Refs. [4,24] we present the results obtained with (QED) and without inclusion of the QED corrections (Breit). Again we see a very good agreement (at the level of a few tenths of a percent) between the theoretical and experimental

TABLE VII. Ti-like W^{52+}. The energies (in cm^{-1}), wavelengths (in nm), and $M1$ transition rates (in s^{-1}) for the states within the $3d^4$ configuration are presented. The results obtained with and without the QED corrections are listed in the columns labeled BREIT and QED. The wavelengths of four lines are compared with the NIST data [1]. Numbers in brackets represent powers of 10.

Transition		Energy (lower level)		Energy (upper level)		Wavelength (nm)			A_{M1} (s^{-1})		
Final	Initial	BREIT	QED	BREIT	QED	BREIT	QED	Ref. [1]	BREIT	QED	Ref. [1]
$^3F_3^2$	$^3D_2^4$	1238038	1241125	2017244	2021769	12.834	12.810		4.32[5]	4.36[5]	
$^3F_3^2$	$^3G_4^3$	1238038	1241125	1984359	1988946	13.399	13.372		1.27[6]	1.28[6]	
$^3F_3^1$	$^5G_4^2$	665288	666894	1402530	1405591	13.564	13.537	13.543	1.10[6]	1.10[6]	1.09[6]
$^3G_4^2$	$^3F_3^4$	1242410	1245550	1978832	1983434	13.579	13.552		1.94[5]	1.97[5]	
$^5F_3^3$	$^3D_2^5$	1724081	1728693	2458818	2464864	13.610	13.584		2.52[6]	2.54[6]	
$^5G_4^1$	$^5F_3^3$	1124398	1127552	1856826	1861430	13.653	13.626		5.77[5]	5.81[5]	
$^5H^5$	$^5G_4^4$	1772951	1777619	2376012	2382140	16.582	16.542		1.28[6]	1.29[6]	
$^5F_3^3$	$^3D_2^5$	1856826	1861430	2458818	2464864	16.612	16.572		8.10[5]	8.16[5]	
$^1D_2^1$	$^5F_3^3$	1255734	1258834	1856826	1861430	16.636	16.595		8.11[5]	8.19[5]	
$^3F_3^2$	$^1D_2^2$	1238038	1241125	1838978	1843576	16.641	16.599		1.86[6]	1.87[6]	
$^3P^1$	$^3D_2^2$	514599	516181	1104742	1107799	16.945	16.903	16.890	4.70[6]	4.74[6]	4.70[6]
$^3P_1^0$	$^5D^0$	514599	516181	1101522	1104648	17.038	16.993		8.16[6]	8.23[6]	
$^5I_6^1$	$^5H^5$	1195327	1198507	1772951	1777619	17.312	17.268		7.92[5]	7.98[5]	
$^3F_3^1$	$^3G_4^2$	665288	666894	1242410	1245550	17.327	17.281		6.27[5]	6.32[5]	
$^5G_4^2$	$^3F_3^4$	1402530	1405591	1978832	1983434	17.352	17.306		1.89[6]	1.90[6]	
$^3D_2^1$	$^1P_1^1$	636589	638203	1211691	1214819	17.388	17.343		3.27[6]	3.30[6]	
$^5F_3^1$	$^5G_4^3$	1140618	1143757	1713475	1718101	17.456	17.411		1.63[6]	1.64[6]	
$^3G_4^1$	$^3H^5$	613414	615007	1171480	1174638	17.919	17.869	17.846	1.65[6]	1.66[6]	1.65[6]
$^3H^5$	$^5G_4^3$	1171480	1174638	1713475	1718101	18.450	18.401		3.46[5]	3.48[5]	
$^3G_4^2$	$^5H^5$	1242410	1245550	1772951	1777619	18.849	18.795		1.41[6]	1.43[6]	
$^5F_3^3$	$^5G_4^4$	1856826	1861430	2376012	2382140	19.261	19.205		3.86[5]	3.89[5]	
$^3P_0^1$	$^3P^1$	0	0	514599	516181	19.433	19.373	19.319	3.31[6]	3.33[6]	3.31[6]
$^3D_2^1$	$^5F_3^1$	636589	638203	1140618	1143757	19.840	19.780		1.38[6]	1.39[6]	
$^3G_4^2$	$^5F_3^3$	1242410	1245550	1724081	1728693	20.761	20.698		3.10[5]	3.13[5]	
$^3F_3^4$	$^3D_2^5$	1978832	1983434	2458818	2464864	20.834	20.771		5.16[5]	5.20[5]	

values. It demonstrates the capabilities of the CI + all-order approach, not observed previously, even for a system with such large number of the valence electrons.

In Table VII we list the energies, transition wavelengths, and the magnetic-dipole transitions rates for 25 transitions in the region 13.3–21.7 nm. The calculated wavelengths are compared with the NIST data where available. The calculation was done in the BREIT and QED approximations. The $M1$ transition rates change by 1% or less, when the QED corrections are included. The results are in good agreement with experiment even for this ion with five valence electrons.

VII. UNCERTAINTIES

There are several distinct sources of uncertainties in our calculations arising from the treatment of the correlation corrections, Breit interaction, and QED contribution:

(i) *Core-valence correlations*. We estimate uncertainties in the core-valence correlations by carrying out a separate calculation of the W^{54+} energies using an approach combining CI with the many-body perturbation theory (CI + MBPT method [34,35]). In this method, the effective Hamiltonian used by the CI is constructed by using the second-order MBPT rather than the all-order linearized coupled-cluster approach, but all other aspects of the calculations are kept the same. The difference of the CI + all-order and CI + MBPT values gives the contribution of the higher orders to core-valence correlations and gives a good estimate of the uncertainty of this contribution. We note that the basis set is the same for all ions computed in this work, so it is sufficient to study this contribution on the example of the W^{54+} ion.
We find that the higher orders contribute from 30 to 1930 cm^{-1} to the energy levels listed in Table I. All energies of the excited states are counted from the ground-state energy. The relative contribution is 0.004%–0.1% for all levels, with the exception of the first-excited level $3d^2\,^3P_0$, whose relative difference is 0.6% (1150 cm^{-1}). Its energy is three times smaller than the energy of the next excited state and a relative role of different corrections for this level is greater than for other levels.

(ii) *Valence correlations*. Usually, we expect that valence-valence correlations can be taken into account with a high accuracy for 2–3 valence-electron systems, because we can make the set of the included configurations essentially complete for a small number of valence electrons. However, we find that a good accuracy can also be achieved even for certain five-valence-electron systems. A main reason for this is that the states belonging to the $3d^n$ configurations are very pure, with little mixing with other states. We see no significant deterioration of the agreement with the experiment for all four ions considered.

(iii) *Breit interaction*. The correction to the Coulomb repulsion between two electrons due to the exchange of a transverse photon is referred to as the Breit interaction (see, e.g., Ref. [36]), which can be represented by the sum of

TABLE VIII. V-like W^{51+} ion. The energies (in cm^{-1}) obtained with and without the QED corrections are compared with the recommended NIST data [26] and theoretical results [4,24]. The first line gives the first ionization potential. The energies of the excited states are counted from the ground-state energy. The nonrelativistic g factor (nr) and g factor obtained using the CI + all-order method (BREIT) are presented.

	Energies (cm^{-1})					g factors	
Level	NIST [26]	FAC [24]	GRASP2K [4]	BREIT	QED	nr	CI + all
$3d^5\ ^2D^1_{5/2}$	37983000			37945680	37948570	1.2000	1.2822
$3d^5\ ^6F^1_{5/2}$	471630	472028	470750	468146	469774	1.3143	1.3318
$3d^5\ ^2F^1_{7/2}$	566250	566411	565800	563903	565494	1.1429	1.1584
$3d^5\ ^2H^1_{11/2}$	577000	577799	576780	576277	577918	1.0909	1.0992
$3d^5\ ^2G^1_{9/2}$	623000	622200	621610	620208	621826	1.1111	1.1305
$3d^5\ ^2D^2_{5/2}$	652000	651268	651450	648810	650413	1.2000	1.1287
$3d^5\ ^4G^1_{7/2}$	688180	687902	688280	687456	689046	0.9841	1.0705
$3d^5\ ^6F^2_{5/2}$	1015000	1029107	1027970	1024098	1027257	1.3143	1.3048
$3d^5\ ^6G_{7/2}$	1097000	1099591	1098610	1094919	1098117	1.1429	1.2076
$3d^5\ ^2H^2_{11/2}$	1103430	1104044	1102510	1100077	1103327	1.0909	1.0866
$3d^5\ ^2G^2_{9/2}$	1118000	1119699	1118700	1115549	1118751	1.1111	1.1395
$3d^5\ ^2I_{13/2}$	1143000	1145266	1143780	1142179	1145455	1.0769	1.0654
$3d^5\ ^4F^1_{5/2}$		1176625	1176610	1172881	1176064	1.0286	1.0181
$3d^5\ ^2G^3_{9/2}$		1219389	1219210	1217160	1220340	1.1111	1.0967
$3d^5\ ^4G^2_{7/2}$		1239133	1239440	1236033	1239226	0.9841	0.9809
$3d^5\ ^4F^2_{5/2}$		1256023	1256460	1253008	1256180	1.0286	1.0455
$3d^5\ ^4G^3_{7/2}$		1308836	1309620	1306521	1309701	0.9841	1.0291
$3d^5\ ^2G^4_{9/2}$		1380571	1381180	1378572	1381728	1.1111	1.1020
$3d^5\ ^2D^3_{5/2}$		1532735	1534710	1531075	1534206	1.2000	1.1796
$3d^5\ ^2D^4_{5/2}$		1664066	1663980	1660296	1665012	1.2000	1.2258
$3d^5\ ^2F^2_{7/2}$		1736600	1736620	1732606	1737371	1.1429	1.1769
$3d^5\ ^6I_{11/2}$		1749908	1749340	1746256	1751069	1.0350	1.0665
$3d^5\ ^2G^5_{9/2}$		1808859	1808950	1804897	1809638	1.1111	1.1105
$3d^5\ ^4F^3_{5/2}$		1845210	1846490	1842989	1847687	1.0286	1.1072
$3d^5\ ^4G^4_{7/2}$		1873738	1874380	1869220	1873952	0.9841	1.0105
$3d^5\ ^2D^5_{5/2}$		2365325	2366700	2361633	2367885	1.2000	1.1479

two terms: the magnetic (Gaunt) term and a two-body term describing retardation effects on the charge-charge interaction. We verified that disregarding the two-body term of the Breit interaction in the basis set and in the CI has negligible effect on the calculation accuracy. Due to very small mixing of the configurations, it is sufficient to study only the difference of the Breit correction to the $3d_{3/2}$ and $3d_{5/2}$ orbitals. An accounting for the Gaunt part of the Breit interaction changes the $3d_{3/2}$–$3d_{5/2}$ splitting by $\sim$15 000 cm^{-1} while further inclusion of the two-body terms adds to this splitting only 85 cm^{-1}, which is negligible at the present level of accuracy. We also omit the two-body Breit interaction when calculating the effective Hamiltonian.

(iv) *QED*. The QED corrections are small for the $3d^n$ states, not exceeding 0.2%, and the resulting uncertainty is negligible (see Ref. [22] for the discussion of the QED uncertainty).

VIII. CONCLUSION

We calculated the energy levels, ionization potentials, wavelengths, and $M1$ and $E2$ transition rates between the states within the $3d^n$ configurations of Ca-, Sc-, Ti-, and V-like W ions by using the CI + all-order method. We summarize the main findings below:

(i) By comparing the energies and wavelengths obtained in this work with those available in the NIST database and other available theoretical results, we found a very good agreement between them. It is worth noting that, in contrast with neutral atoms, the calculation accuracy is practically the same for divalent and multivalent highly charged ions. This is because the main configuration of a considered state typically gives a dominating contribution ($\sim$98% in probability or even more) and the configuration mixing does not play for HCIs a substantial role. For this reason there is no loss of accuracy at the CI stage for multivalent ions in comparison with the divalent ones. This significantly extends a range of applicability of the CI + all-order method to HCIs and provides first demonstration of its accuracy for a system with five valence electrons.

(ii) We analyzed the role of the QED corrections and found that they are small for $3d^n$ configuration but significant when high-precision results are needed.

(iii) We calculated the transition rates between selected states of the ions listed above. We observed that the $M1$ transition rates (when they are allowed by selection rules) completely dominate for the transitions within the $3d^n$ configurations while the $E2$ transition rates for the same transitions are few orders of magnitude smaller. There is excellent agreement between our $M1$ transition rates and the NIST data [1].

TABLE IX. V-like W^{51+}. The energies (in cm^{-1}), wavelengths (in nm), and $M1$ transition rates (in s^{-1}) for the states belonging to the $3d^4$ configuration. In the columns labeled BREIT and QED the results obtained with and without the QED corrections are listed in the QED and BREIT columns, respectively. The wavelengths and $M1$ rates of five transitions are compared with the NIST data [1].

Transition		Energy (lower level)		Energy (upper level)		Wavelength (nm)			A_{M1} (s^{-1})		
Final	Initial	BREIT	QED	BREIT	QED	BREIT	QED	Ref. [1]	BREIT	QED	Ref. [1]
$^6G_{7/2}$	$^4F^3_{5/2}$	1094919	1098117	1842989	1847687	13.368	13.341		1.53[6]	1.54[6]	
$^6G_{7/2}$	$^2G^5_{9/2}$	1094919	1098117	1804897	1809638	14.085	14.054		1.05[6]	1.06[6]	
$^2D^4_{5/2}$	$^2D^5_{5/2}$	1660296	1665012	2361633	2367885	14.258	14.227		6.47[6]	6.52[6]	
$^4F^1_{5/2}$	$^4G^4_{7/2}$	1172881	1176064	1869220	1873952	14.361	14.329		3.06[5]	3.09[5]	
$^4G^1_{7/2}$	$^2G^4_{9/2}$	687456	689046	1378572	1381728	14.469	14.437		1.09[6]	1.09[6]	
$^2F^1_{7/2}$	$^4F^2_{5/2}$	563903	565494	1253008	1256180	14.512	14.478	14.531	1.57[6]	1.58[6]	1.21[6]
$^4F^1_{5/2}$	$^4F^3_{5/2}$	1172881	1176064	1842989	1847687	14.923	14.889		1.72[6]	1.73[6]	
$^2H^2_{11/2}$	$^6I_{11/2}$	1100077	1103327	1746256	1751069	15.476	15.438		3.45[6]	3.48[6]	
$^6G_{7/2}$	$^2F^2_{7/2}$	1094919	1098117	1732606	1737371	15.682	15.643		2.14[6]	2.15[6]	
$^2G^2_{9/2}$	$^6I_{11/2}$	1115549	1118751	1746256	1751069	15.855	15.815		1.03[6]	1.04[6]	
$^4G^1_{7/2}$	$^4G^3_{7/2}$	687456	689046	1306521	1309701	16.153	16.112		1.01[6]	1.02[6]	
$^2G^2_{9/2}$	$^2F^2_{7/2}$	1115549	1118751	1732606	1737371	16.206	16.165		2.64[6]	2.66[6]	
$^2F^1_{7/2}$	$^4F^1_{5/2}$	563903	565494	1172881	1176064	16.421	16.378		1.29[6]	1.30[6]	
$^2G^1_{9/2}$	$^2G^3_{9/2}$	620208	621826	1217160	1220340	16.752	16.708		2.58[6]	2.60[6]	
$^4F^2_{5/2}$	$^4F^3_{5/2}$	1253008	1256180	1842989	1847687	16.950	16.906		2.78[5]	2.80[5]	
$^4G^2_{7/2}$	$^2G^5_{9/2}$	1236033	1239226	1804897	1809638	17.579	17.531		7.09[5]	7.14[5]	
$^2H^1_{11/2}$	$^2I_{13/2}$	576277	577918	1142179	1145455	17.671	17.620		5.18[5]	5.23[5]	
$^4G^1_{7/2}$	$^4F^2_{5/2}$	687456	689046	1253008	1256180	17.682	17.633		1.50[6]	1.51[6]	
$^6G_{7/2}$	$^2D^4_{5/2}$	1094919	1098117	1660296	1665012	17.687	17.640		1.73[6]	1.75[6]	
$^2D^1_{5/2}$	$^2F^1_{7/2}$	0	0	563903	565494	17.734	17.684	17.660	1.60[6]	1.61[6]	1.59[6]
$^4F^1_{5/2}$	$^2F^2_{7/2}$	1172881	1176064	1732606	1737371	17.866	17.816		1.22[6]	1.23[6]	
$^6F^1_{5/2}$	$^6F^2_{5/2}$	468146	469774	1024098	1027257	17.987	17.938		6.55[6]	6.62[6]	
$^2F^1_{7/2}$	$^2G^2_{9/2}$	563903	565494	1115549	1118751	18.128	18.075		1.41[6]	1.42[6]	
$^4G^1_{7/2}$	$^4G^2_{7/2}$	687456	689046	1236033	1239226	18.229	18.176		4.24[5]	4.28[5]	
$^2D^2_{5/2}$	$^4F^1_{5/2}$	648810	650413	1172881	1176064	19.081	19.024		1.41[6]	1.42[6]	
$^2H^1_{11/2}$	$^2H^2_{11/2}$	576277	577918	1100077	1103327	19.091	19.033	18.996	2.31[6]	2.33[6]	2.31[6]
$^2G^3_{9/2}$	$^2F^2_{7/2}$	1217160	1220340	1732606	1737371	19.401	19.341		5.63[5]	5.68[5]	
$^2G^1_{9/2}$	$^6G_{7/2}$	620208	621826	1094919	1098117	21.065	20.996		9.19[5]	9.26[5]	
$^2D^1_{5/2}$	$^6F^1_{5/2}$	0	0	468146	469774	21.361	21.287	21.203	3.38[6]	3.42[6]	3.40[6]
$^2F^1_{7/2}$	$^6F^2_{5/2}$	563903	565494	1024098	1027257	21.730	21.656		5.02[5]	5.07[5]	

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