

Atomic properties of Cd-like and Sn-like ions for the development of frequency standards and search for the variation of the fine-structure constant

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A high-precision relativistic calculation of Cd-like Nd^{12+} , Sm^{14+} and Sn-like Pr^{9+} , Nd^{10+} atomic properties is carried out using an approach that combines configuration interaction and a linearized coupled-cluster method. These ions have long-lived metastable states with transitions accessible by laser excitations, relatively simple electronic structure, high sensitivity to α variation, and stable isotopes. Breit and QED corrections were included into the calculations. Energies, transition wavelengths, electric- and magnetic-multipole reduced matrix elements, lifetimes, and sensitivity coefficients q and K to the variation of the fine-structure constant α were obtained. A detailed study of uncertainties was performed. Energies for similar Cd-like Ba^{8+} , La^{9+} , Ce^{10+} , Pr^{11+} and Sn-like Ba^{6+} ions were calculated and compared with experiment for further tests of the accuracy.

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I. INTRODUCTION

The past five years marked extraordinary improvements in both the accuracy and stability of optical frequency standards [1–3]. The most accurate trapped-ion clock based on quantum logic spectroscopy of an Al^+ ion was demonstrated in 2010 [1]. The fractional frequency uncertainty of 8.6×10^{-18} was reported. The optical frequency standard based on $^{88}\text{Sr}^+$ trapped ion with the total fractional frequency uncertainty of 2.3×10^{-17} was reported in [4]. In 2013, Yb lattice clock with instability of 8.6×10^{-18} after only 7 h of averaging [2] was reported. The 6.4×10^{-18} accuracy was achieved with the Sr optical lattice clock [3] which represents a factor of 22 improvement in comparison with the best previous optical lattice clock. Cryogenic Sr optical lattice clocks with a relative frequency difference of 10^{-18} was demonstrated in [5].

Further development of even more precise frequency standards is essential for new tests of fundamental physics, search for the variation of fundamental constants, and very-long-baseline interferometry for telescope array synchronization. The most precise laboratory test of variation of the fine-structure constant α has been carried out by measuring the frequency ratio of Al^+ and Hg^+ optical atomic clocks with a fractional uncertainty of 5.2×10^{-17} [6]. Furthermore, more precise clocks will enable the development of extremely sensitive quantum-based tools for geodesy, hydrology, climate change studies, inertial navigation, and tracking of deep-space probes [2,3].

This remarkable progress poses the question of what are the novel schemes for the clock development that may achieve the accuracy at the next decimal point, 10^{-19} . We can single out two types of new clock scheme proposals at the present time. The first set of proposals are for the development of a nuclear clock [7] based on the ^{229}Th nuclear transition that has an unusually low first excitation energy of only several eV making it accessible with laser excitation. The second set of proposals

involves various transitions in highly charged ions (HCI) [8–10]. The estimates of potential accuracy of clocks based on highly charged ions and the ^{229}Th nuclear transition are similar, but most HCI clock proposals do not have a complication of dealing with the radioactive isotope.

Recent studies of uncertainties [9,10] have shown that the fractional uncertainty of the transition frequency in the clocks based on HCIs can be smaller than 10^{-19} . Estimated sensitivity to the variation of α for highly charged ions approaches 10^{-20} per yr [10], which may allow for tests of spatial variation of the fine-structure constant that may be indicated by the observational studies [11].

While HCIs lack strong electric-dipole transitions for laser cooling, some have strong $M1$ transitions. Moreover, sympathetic cooling may be employed similar to the scheme used in Al^+ clock, which is cooled using laser-cooled Be^+ or Mg^+ ions [1]. The experimental investigations toward the sympathetic cooling of HCIs and the precision laser spectroscopy of forbidden transitions are in progress [12–15]. A cooling scheme combining laser cooling of Be^+ ions and sympathetic cooling of Xe^{44+} by Coulomb collisions with the cold Be^+ ions has been demonstrated in [16]. In 2011, the evaporative cooling of Ar^{16+} in a Penning trap was demonstrated [12]. A novel extraction technique based on the excitation of a coherent axial oscillation which allowed one to monitor the cooling process and to extract HCI bunches of high density and low momentum spread was also demonstrated [12]. Laser cooling of Mg^+ ions in a Penning trap for sympathetic cooling of highly charged ions was demonstrated in [13]. Storage and cooling of highly charged ions require ultrahigh vacuum levels. These can be obtained by cryogenic methods, and a linear Paul trap operating at 4 K capable of very long ion storage times of about 30 h was recently developed in [14,15]. Capture and isolation of highly charged ions in a unitary Penning trap extracted from an electron beam ion trap (EBIT) at NIST was demonstrated in [17]. The observed energy distribution was

60 times smaller than typically expected for ions inside an EBIT without applying any active cooling [17].

In a recent work, we proposed 10 highly charged ions that belong to Ag-like, In-like, Cd-like, and Sn-like isoelectronic sequences as candidates for the development of next generation atomic clocks, search for variation of fine-structure constant, and quantum information [18]. Ag-like and In-like highly charged ions have been further considered in Ref. [19].

In this work, we carried out a detailed high-precision study of Cd-like Nd^{12+} , Sm^{14+} and Sn-like Pr^{9+} , Nd^{10+} highly charged ions using an approach that combines configuration interaction (CI) and a variant of the coupled-cluster method. Breit and quantum electrodynamic (QED) corrections were included into the calculations. Our calculations include energies, transition wavelengths, electric-dipole, electric-quadrupole, electric-octupole, magnetic-dipole, magnetic-quadrupole, magnetic-octupole reduced-matrix elements, lifetimes, and sensitivity coefficients to α -variation q and K . We carried out extensive study of the uncertainties of our results. Two types of calculations were carried out for Sn-like ions, treating these ions as systems with two- and four-valence

electrons to ensure that all important configurations were taken into account. Energies for similar Cd-like Ba^{8+} , La^{9+} , Ce^{10+} , Pr^{11+} and Sn-like Ba^{6+} ions, where the experimental values are available, were calculated and compared with experiment for further tests of accuracy. Our values are in excellent agreement with experimental energies from [20–22] for Cd-like Ba^{8+} , La^{9+} , Ce^{10+} , with similar level of agreement for all three ions. However, we find a significant discrepancy with experimental values from [23,24] for Pr^{11+} and Nd^{12+} which might indicate a problem with the experimental level identification. Detailed study of higher-order, Breit, QED, and higher partial-wave contributions was carried out to evaluate uncertainties of the final results for each ion.

We start with the brief description of the CI+all-order method used in this work in Sec. II. The results for Cd-like and Sn-like ions are presented in Secs. III and IV, respectively.

II. METHOD

The Cd-like ions are divalent systems with two-valence electrons above the $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6 4d^{10}$ core.

TABLE I. Energies of Cd-like Ba^{8+} , Nd^{12+} , and Sm^{14+} ions relative to their ground states evaluated using the CI+all-order method (in cm^{-1}). Contributions from higher-order Coulomb correlation (difference of the CI+all-order and CI+MBPT calculation), estimated contributions of higher partial waves ($l > 6$), the Breit, and QED corrections are given separately in columns HO, Extrap, Breit, and QED. Experimental results are from [20] for Ba^{8+} and [24] for Nd^{12+} . Difference with experiment is given in cm^{-1} and % in columns “Diff.” Estimated absolute uncertainties of theoretical calculations are given in columns “Unc.” Theoretical and experimental wavelengths for transitions to the ground states are given in the last two columns in nm.

Ion	Level	Expt.	CI+MBPT	HO	Extrap	Breit	QED	Final	Unc	Diff.	Diff.%	λ_{theor}	λ_{expt}
Ba^{8+}	$5s^2 \ ^1S_0$	0	0	0	0	0	0	0					
	$5s5p \ ^3P_0$	116992	119350	−1434	1	349	−506	117760		−768	−0.66%	84.92	85.48
	$5s5p \ ^3P_1$	122812	124971	−1289	3	298	−500	123483		−671	−0.55%	80.98	81.43
	$5s5p \ ^3P_2$	142812	145610	−1532	13	25	−461	143655		−843	−0.59%	69.61	70.02
	$5s5p \ ^1P_1$	175712	175440	646	21	33	−466	175674		38	0.02%	56.92	56.91
	$4f5s \ ^3F_2$	237170	238470	809	−898	−912	−558	236911		259	0.11%	42.21	42.16
	$4f5s \ ^3F_3$	237691	239062	792	−896	−971	−555	237432		259	0.11%	42.12	42.07
	$4f5s \ ^3F_4$	238547	240038	755	−891	−1078	−548	238276		271	0.11%	41.97	41.92
	$4f5s \ ^1F_3$	245192	246989	768	−900	−1033	−566	245258		−66	−0.03%	40.77	40.78
Nd^{12+}	$5s^2 \ ^1S_0$	0	0	0	0	0	0	0					
	$5s4f \ ^3F_2$	77162	81730	1258	−1128	−1407	−983	79469	600	2307	2.99%	125.8(9)	129.6
	$5s4f \ ^3F_3$	78443	83119	1246	−1127	−1489	−979	80769	610	2326	2.97%	123.8(9)	127.5
	$5s4f \ ^3F_4$	81440	86393	1198	−1121	−1763	−978	83730	650	2290	2.81%	119.4(9)	122.8
	$5s4f \ ^1F_3$	87312	92519	1218	−1128	−1699	−959	89951	640	2639	3.02%	111.2(8)	114.5
	$5s5p \ ^3P_0$	156417	161505	−1511	−7	650	−970	159667	1020	3250	2.08%	62.6(4)	63.9
	$5s5p \ ^3P_1$	165482	170161	−1223	−5	584	−970	168547	800	3065	1.85%	59.3(3)	60.4
	$5s5p \ ^3P_2$	204685	210480	−1620	8	77	−970	207976	1400	3291	1.61%	48.1(3)	48.9
	$5s5p \ ^1P_1$	245748	245644	821	16	83	−970	245594	320	−154	−0.06%	40.7(1)	40.7
Sm^{14+}	$4f^2 \ ^3H_4$		0	0	0	0	0	0					
	$5s4f \ ^3F_2$		611	−2437	1140	1658	1201	2172	850			4600(1300)	
	$5s4f \ ^3F_3$		2355	−2447	1140	1574	1204	3826	840			2614(470)	
	$4f^2 \ ^3H_5$		5378	−61	4	−408	26	4939	100			2025(40)	
	$5s4f \ ^3F_4$		7392	−2498	1146	1190	1233	8463	810			1182(100)	
	$4f^2 \ ^3F_2$		9320	−194	40	35	6	9207	50			1086(6)	
	$4f^2 \ ^3H_6$		10797	−124	9	−827	51	9906	210			1010(20)	
	$4f^2 \ ^3F_3$		12974	−235	39	−274	27	12532	90			798(6)	
	$4f^2 \ ^1G_4$		13620	−223	36	−352	26	13108	110			763(6)	
	$5s4f \ ^1F_3$		13207	−2479	1141	1254	1214	14337	810			698(40)	
	$4f^2 \ ^3F_4$		20633	−299	43	−715	56	19717	200			507(5)	

TABLE II. Comparison of theoretical energies with experiment for Cd-like Ba⁸⁺ [20], La⁹⁺ [21], Ce¹⁰⁺ [22], Pr¹¹⁺ [23], and Nd¹²⁺ [24] ions relative to the 5s² ¹S₀ ground state (in cm⁻¹). Actual (in cm⁻¹) and relative (in %) differences with experiment are given for all states. The states are listed in the same order for all ions. Fine-structure intervals for 5s5p and 4f5s triplets are listed in the last four rows.

Level	Ba ⁸⁺			La ⁹⁺			Ce ¹⁰⁺			Pr ¹¹⁺			Nd ¹²⁺		
	Theory	Diff.	%	Theory	Diff.	%	Theory	Diff.	%	Theory	Diff.	%	Theory	Diff.	%
5s5p ³ P ₀	117760	-768	-0.7	128226	-811	-0.6	138718	-867	-0.6	149252	-2934	-2.0	159667	-3250	-2.1
5s5p ³ P ₁	23483	-671	-0.6	134719	-697	-0.5	145996	-729	-0.5	157329	-2774	-1.8	168547	-3065	-1.9
5s5p ³ P ₂	143655	-843	-0.6	158956	-885	-0.6	173838	-891	-0.5	191188	-3020	-1.6	207976	-3291	-1.6
5s5p ¹ P ₁	175674	38	0.0	192451	33	0.0	209702	1	0.0	227471	-24	-0.0	245594	154	0.1
4f5s ³ F ₂	236911	259	0.1	207147	165	0.1	170661	41	0.0	127955	-1969	-1.6	79469	-2307	-3.0
4f5s ³ F ₃	237432	259	0.1	207865	159	0.1	171521	91	0.1	129067	-1984	-1.6	80769	-2326	-3.0
4f5s ³ F ₄	238276	271	0.1	209118	171	0.1	173364	104	0.1	131378	-1964	-1.5	83730	-2290	-2.8
4f5s ¹ F ₃	245258	-66	-0.0	215933	-144	-0.1	179860	-232	-0.1	137767	-2297	-1.7	89951	-2639	-3.0
³ P ₁ - ³ P ₀	5723	97	1.7	6493	114	1.7	7278	138	1.9	8077	160	1.9	8880	185	2.0
³ P ₂ - ³ P ₁	20172	-172	-0.9	24237	-188	-0.8	28571	-162	-0.6	33859	-246	-0.7	39429	-226	-0.6
³ F ₃ - ³ F ₂	521	0	0.0	718	-6	-0.8	860	50	5.5	1112	-15	-1.4	1300	-19	-1.5
³ F ₄ - ³ F ₃	844	12	1.4	1253	12	1.0	1752	13	0.7	2311	20	0.9	2961	36	1.2

We use a CI+all-order method developed in [25,26] that combines the modified linearized single-double coupled-cluster approach with configuration interaction. The CI many-electron wave function is obtained as a linear combination of all distinct states of a given angular momentum J and parity [27]:

$$\Psi_J = \sum_i c_i \Phi_i. \quad (1)$$

The CI+many-body perturbation theory (MBPT) approach developed in [28] allows one to incorporate core excitations in the CI method by including perturbation theory terms into an effective Hamiltonian H^{eff} . The one-body part H_1 is modified to include the correlation potential Σ_1 that accounts for one-body part of the core-valence correlations:

$$H_1 \rightarrow H_1 + \Sigma_1 \quad (2)$$

and the two-body Coulomb interaction term H_2 is modified by including the two-body part of core-valence interaction that represents screening of the Coulomb interaction by valence electrons:

$$H_2 \rightarrow H_2 + \Sigma_2. \quad (3)$$

Then, the energies and wave functions of low-lying states are determined by diagonalizing the effective Hamiltonian:

$$H^{\text{eff}} = H_1 + H_2, \quad (4)$$

where H_1 and H_2 are modified according to Eqs. (2) and (3). The matrix elements and other properties, such as polarizabilities, can be determined using the resulting wave functions [27].

In the CI+all-order approach, the corrections to the effective Hamiltonian Σ_1 and Σ_2 are calculated using a modified version of the linearized coupled-cluster all-order method which allows one to include dominant core and core-valence correlation corrections to the effective Hamiltonian to all orders and improve accuracy in comparison with the CI+MBPT method. The detailed description of the CI+all-order method and all formulas are given in [26].

When the CI space includes only two or three electrons, it can be made essentially complete. For four-electron systems,

we have developed an efficient algorithm to construct a sufficiently complete set of configurations. The CI+all-order method yielded accurate wave functions for calculations of such atomic properties as lifetimes, polarizabilities, hyperfine-structure constants, etc., for a number of divalent and trivalent systems [26,29–35]. The spectra of the superheavy elements No, Lr, and Rf with two-, three-, and four-valence electrons were recently presented by Dzuba *et al.* [36].

We included the Breit interaction on the same footing as the Coulomb interaction at the stage of constructing the basis set, and incorporated the Gaunt part of the Breit interaction in the CI. The QED radiative corrections to the energy levels are included using the method described in [37]. We find the QED contribution to be significant only for the configurations that contain valence 5s state, and omit it for Sn-like ions where none

TABLE III. Transition energies ω and sensitivity coefficients q for Cd-like ions relative to the ground state evaluated using the CI+all-order method in cm⁻¹; $K = 2q/\omega$ is the enhancement factor.

Ion	Level	ω	q	K
Nd ¹²⁺	5s ² ¹ S ₀	0	0	
	5s4f ³ F ₂	79469	101461	2.6
	5s4f ³ F ₃	80769	102325	2.5
	5s4f ³ F ₄	83730	105340	2.5
	5s4f ¹ F ₃	89951	105827	2.4
	5s5p ³ P ₀	159667	14175	0.2
	5s5p ³ P ₁	168547	19465	0.2
Sm ¹⁴⁺	4f ² ³ H ₄	0	0	
	5s4f ³ F ₂	2172	-127720	-118
	5s4f ³ F ₃	3826	-126746	-66
	4f ² ³ H ₅	4939	4917	2.0
	5s4f ³ F ₄	8463	-121952	-29
	4f ² ³ F ₂	9207	1324	0.3
	4f ² ³ H ₆	9906	9295	1.9
	4f ² ³ F ₃	12532	4954	0.8
	4f ² ¹ G ₄	13108	4508	0.7
	5s4f ¹ F ₃	14337	-121525	-17
	4f ² ³ F ₄	19717	10045	1.0

of the low-lying configurations contain $5s$ valence electron. The partial waves with $l_{\max} = 6$ are included in all summations in many-body perturbation theory or coupled-cluster terms. Extrapolation of the $l > 6$ contribution is carried out following the method described in Ref. [19].

The lifetime of a state a is calculated as

$$\tau_a = \frac{1}{\sum_b A_{ab}}, \quad (5)$$

where the multipole transition rates A_{ab} are related to the line strengths S_{ab} . Explicit expressions are given in Ref. [19]. In the sum (5) we account for the electric (E_k) and magnetic (M_k) transitions of the ranks $k = 1-3$.

The sensitivity of the atomic transition frequency ω to the variation of the fine-structure constant α can be quantified

using a coefficient q defined as $\omega(x) = \omega_0 + qx$, where $x \equiv (\frac{\alpha}{\alpha_0})^2 - 1$ and the frequency ω_0 corresponds to the value of the fine-structure constant α_0 at some initial point in time. It is convenient to also define dimensionless enhancement factor $K = 2q/\omega$. We follow the same procedure to calculate q as in Ref. [19]. Briefly, we carry out three calculations with different values of α for every ion considered in this work. In the first calculation, current CODATA value of α [38] is used. In the other two calculations, the value of α^2 is varied by $\pm 1\%$. The value of q is then determined as a numerical derivative.

III. CD-LIKE IONS

The $5s-4f$ level crossing in Cd-like ions happens for Nd^{12+} – Sm^{14+} ions. The order of levels in previous ions of the

TABLE IV. CI+all-order multipole reduced matrix elements Z (in a.u.), transition rates A_r (in s^{-1}), and lifetimes τ (in sec) in Cd-like Nd^{12+} and Sm^{14+} ions. Transition energies (in cm^{-1}) and corresponding wavelengths (in nm) are obtained from the theoretical energies given in Table I. The numbers in brackets represent powers of 10.

Ion	Level	Transition		Energy	λ	Z	A_r	τ		
Nd^{12+}	$5s4f\ ^3F_2$	$5s2\ ^1S_0$	$5s4f\ ^3F_2$	$M2$	79469	125.8	0.00012	1.312[−11]	7.622[+10]	
		$5s4f\ ^3F_3$	$5s4f\ ^3F_3$	$M1$	1300	7692	2.49401	5.266[−02]	18.90	
	$5s4f\ ^3F_4$	$5s4f\ ^3F_3$	$5s4f\ ^3F_4$	$M1$	2961	3377	2.50909	4.898[−01]	2.042	
		$5s4f\ ^3F_2$	$5s4f\ ^3F_4$	$E2$	4261	2347	0.07926	1.098[−07]		
	$5s4f\ ^1F_3$	$5s4f\ ^3F_2$	$5s4f\ ^1F_3$	$M1$	10482	954.0	0.61326	1.669[+00]	0.410	
		$5s4f\ ^3F_4$	$5s4f\ ^1F_3$	$M1$	6221	1607	0.61858	3.549[−01]		
	$5s5p\ ^3P_0$	$5s4f\ ^3F_2$	$5s5p\ ^3P_0$	$E2$	80198	124.7	0.58339	1.265[+02]	7.905[−03]	
		$5s2\ ^1S_0$	$5s5p\ ^3P_1$	$E1$	168547	59.3	0.42601	5.868[+08]	1.710[−09]	
	$5s5p\ ^3P_1$	$5s4f\ ^3F_4$	$5s5p\ ^3P_2$	$E2$	124246	80.5	1.14090	8.632[+02]	6.054[−04]	
		$5s2\ ^1S_0$	$5s5p\ ^3P_2$	$M2$	207976	48.1	5.97200	4.138[+00]		
	$5s5p\ ^3P_2$	$5s4f\ ^3F_2$	$5s5p\ ^3P_2$	$E2$	128507	77.8	0.21718	3.703[+01]		
		$5s5p\ ^3P_0$	$5s5p\ ^3P_2$	$E2$	48309	207.0	1.23160	8.940[+00]		
	$5s5p\ ^3P_1$	$5s5p\ ^3P_1$	$5s5p\ ^3P_2$	$M1$	39429	253.6	1.49436	7.384[+02]		
		$5s2\ ^1S_0$	$5s5p\ ^1P_1$	$E1$	245594	40.7	1.39510	1.947[+10]	5.136[−11]	
	$5s5p\ ^1P_1$	$5s4f\ ^1F_3$	$5s5p\ ^1P_1$	$E2$	155643	64.2	0.89639	2.740[+03]		
		$5s5p\ ^3P_0$	$5s5p\ ^1P_1$	$M1$	85927	116.4	0.42382	1.024[+03]		
			$5s5p\ ^3P_2$	$5s5p\ ^1P_1$	$M1$	37618	265.8	0.47796	1.093[+02]	
	Sm^{14+}	$4f5s\ ^3F_2$	$4f2\ ^3H_4$	$4f5s\ ^3F_2$	$M2$	2172	4604	0.03516	1.782[−14]	5.613[+13]
			$4f2\ ^3H_4$	$4f5s\ ^3F_3$	$E1$	3826	2614	0.00092	1.366[−02]	8.514
		$4f5s\ ^3F_3$	$4f5s\ ^3F_2$	$4f5s\ ^3F_3$	$M1$	1654	6046	2.43986	1.038[−01]	
$4f2\ ^3H_5$			$4f2\ ^3H_5$	$M1$	4939	2025	3.19913	3.024[+00]	0.331	
$4f5s\ ^3F_4$		$4f5s\ ^3F_3$	$4f5s\ ^3F_4$	$M1$	4637	2157	2.45429	1.800[+00]	0.556	
		$4f2\ ^3F_2$	$4f2\ ^3F_2$	$E1$	5381	1858	0.00652	2.682[+00]	0.373	
$4f2\ ^3F_2$		$4f2\ ^3H_4$	$4f2\ ^3F_2$	$E2$	9207	1086	0.49808	3.676[−04]		
		$4f2\ ^3H_5$	$4f2\ ^3H_6$	$M1$	4967	2013	3.26426	2.709[+00]	0.369	
$4f2\ ^3H_6$		$4f5s\ ^3F_2$	$4f2\ ^3F_3$	$E1$	10360	965	0.00205	1.351[+00]	0.328	
		$4f5s\ ^3F_4$	$4f2\ ^3F_3$	$E1$	4069	2458	0.00601	7.041[−01]		
$4f2\ ^3F_3$		$4f2\ ^3F_2$	$4f2\ ^3F_3$	$M1$	3325	3007	2.52457	9.028[−01]		
		$4f2\ ^3H_4$	$4f2\ ^3F_3$	$M1$	12532	798	0.10761	8.782[−02]		
$4f2\ ^1G_4$		$4f5s\ ^3F_3$	$4f2\ ^1G_4$	$E1$	9282	1077	0.00373	2.506[+00]	0.338	
		$4f2\ ^3H_5$	$4f2\ ^1G_4$	$M1$	8169	1224	0.52656	4.530[−01]		
$4f5s\ ^1F_3$		$4f2\ ^3F_3$	$4f2\ ^1G_4$	$M1$	576	17361	1.95991	2.200[−03]		
		$4f2\ ^3H_4$	$4f5s\ ^1F_3$	$E1$	14337	698	0.00475	1.929[+01]	0.0410	
$4f5s\ ^3F_2$		$4f5s\ ^3F_2$	$4f5s\ ^1F_3$	$M1$	12165	822	0.80183	4.460[+00]		
		$4f5s\ ^3F_4$	$4f5s\ ^1F_3$	$M1$	5874	1702	0.80877	5.108[−01]		
$4f2\ ^3F_4$		$4f2\ ^3F_4$	$4f5s\ ^1F_3$	$E1$	1229	8137	0.01529	1.255[−01]		
		$4f5s\ ^1F_3$	$4f2\ ^3F_4$	$E1$	5380	1859	0.01635	9.374[+00]	0.0648	
$4f2\ ^3F_4$	$4f5s\ ^3F_3$	$4f2\ ^3F_4$	$E1$	15891	629	0.00120	1.309[+00]			
	$4f2\ ^3H_5$	$4f2\ ^3F_4$	$M1$	14778	677	0.40844	1.614[+00]			
	$4f2\ ^3F_3$	$4f2\ ^3F_4$	$M1$	7185	1392	1.67986	3.137[+00]			

Cd-like isoelectronic sequence, such as Ba⁸⁺, is 5s², 5s5p, and 5s4f. It changes to 5s², 5s4f, and 5s5p for Nd¹²⁺. The 4f² becomes the ground state for Sm¹⁴⁺, with other low-lying levels belonging to either 4f² or 5s4f configurations. In order to evaluate the uncertainties of our values, we carried out several calculations which allowed us to separate the effect of higher orders, Breit interaction, contributions of higher partial waves, and QED. The contribution of the higher orders is evaluated as the difference of the CI+all-order and CI+MBPT results. The Breit and QED contributions are calculated as the difference of the results with and without the inclusion of these effects. The contribution of the higher (*l* > 6) partial waves (labeled “Extrap”) is estimated to be equal to the contribution of the *l* = 6 partial wave following our empiric rule obtained for Ag-like ions (see [19] for a detailed discussion of the extrapolation). The contribution of the *l* = 6 partial wave is obtained as the difference of two calculations where all intermediate sums in the all-order and MBPT terms are restricted to *l*_{max} = 6 and *l*_{max} = 5. The resulting four contributions are listed separately in Table I. The final theoretical results are listed in the “Final” column.

We develop several methods to estimate the accuracy of our calculations. First, we assume that the uncertainty of each of the four corrections (HO, Extrap, Breit, and QED) does not exceed 25%, and add 25% of each correction in quadrature to estimate the total uncertainty. In Ag-like and In-like ions, such estimates are significantly larger (by a factor 2–4) than our actual difference with the experiment for all three ions

listed in Table I of [18]. For Ba⁸⁺ 5s4f states, which are of most interest for the present work, such an estimate gives about 400 cm⁻¹, while our differences with experiment are 70–270 cm⁻¹. Therefore, we can expect that such a procedure will give reasonable estimates of uncertainties for the 5s4f states of Nd¹²⁺.

In the second approach of evaluating the uncertainties, we use the reference ion, Ba⁸⁺, to estimate the uncertainties in the calculations for the other ion. We estimate the uncertainty as the sum of the following: (1) difference of the theoretical and experimental energies for the reference ion and (2) difference in the sum of all four corrections between the reference and the current ion. For the 5s5p states of Nd¹²⁺, we use this second approach to estimate the uncertainties and also find that these estimates are significantly smaller than our difference with the experiment.

The agreement of the 5s4f energies with the experiment [20] for Ba⁸⁺ is excellent and is of the same relative magnitude (0.1%) as in the case of 4f states of Ag-like Ba⁹⁺ ion. The 5s5p energies agree with experiment to about 0.6%. However, the differences with the experiment for Nd¹²⁺ [24] energies are anomalously large, 1.6%–3% for all states listed in Table I except 5s5p ¹P₁ which is in excellent agreement with experiment. These differences are much larger than our estimated upper bound on the uncertainty of our results listed in column “Unc.”

To explore the discrepancy of our energies with experiment for Nd¹²⁺, we calculated the energies of the other three

TABLE V. Comparison of CI+all-order energies of Sn-like Ba⁶⁺, Pr⁹⁺, and Nd¹⁰⁺ ions relative to the ground state calculated as two-valence-electron (2-valence) and four-valence-electron (4-valence) systems (in cm⁻¹). In the two-valence electron calculation, the 5s shell is taken to be a core shell. Contributions from higher-order Coulomb correlation (difference of the CI+all-order and CI+MBPT calculations), estimated contributions of higher partial waves (*l* > 6), and Breit corrections are given separately in columns labeled “HO,” “Extrap,” and “Breit.” Differences between “4-valence” and “2-valence” final values are given in the last column.

Ion	Term	<i>J</i>	2-valence calculation					4-valence calculation					Diff.	
			CI+MBPT	HO	Extrap	Breit	Final	CI+MBPT	HO	Extrap	Breit	Final		
Ba ⁶⁺	5p ²	³ P ₀	0	0	0	0	0	0	0	0	0	0	0	0
	5p ²	³ P ₁	15554	153	13	-242	15477	15704	-103	10	-238	15372	-105	
	5p ²	³ P ₂	21228	187	13	-267	21161	21788	-108	9	-268	21422	261	
	5p ²	¹ D ₂	42400	-26	24	-510	41888	43143	-233	17	-507	42420	532	
	5p ²	¹ S ₀	62976	-1466	25	-505	61030	62342	-260	21	-501	61602	572	
Pr ⁹⁺	5p ²	³ P ₀	0	0	0	0	0	0	0	0	0	0	0	0
	5p4f	³ G ₃	20050	2994	-1078	-1750	20216	21865	2810	-1032	-1748	21895	1679	
	5p4f	³ F ₂	22664	2489	-862	-1519	22772	24172	2291	-829	-1435	24199	1427	
	5p4f	³ F ₃	25607	2844	-1072	-2017	25362	27233	2804	-1026	-2009	27002	1640	
	5p4f	³ F ₄	27727	2943	-1080	-2054	27536	29622	2801	-1033	-2048	29343	1806	
	5p ²	³ P ₁	28712	193	16	-409	28512	28962	-135	14	-405	28436	-76	
	5p ²	³ P ₂	35831	856	-252	-782	35653	36697	615	-243	-852	36217	564	
	5p4f	¹ F ₃	54104	2728	-1066	-2179	53588	55735	2680	-1023	-2172	55220	1632	
Nd ¹⁰⁺	4f ²	³ H ₄	0	0	0	0	0	0	0	0	0	0	0	0
	5p4f	⁵ G ₃	2605	-4037	1076	1920	1564	1953	-4305	1025	1887	560	-1004	
	4f ²	³ H ₅	3432	-80	1	-294	3059	3405	-58	2	-291	3058	-1	
	5p4f	¹ D ₂	5975	-3629	1009	1704	5060	5171	-3823	923	1768	4040	-1020	
	4f ²	³ H ₆	6982	-167	6	-599	6222	6930	-128	8	-590	6219	-3	
	5p4f	³ F ₃	8448	-3861	1037	1471	7095	7853	-4222	1063	1687	6382	-713	
	4f ² + 5p4f	³ F ₂	8263	-694	113	231	7914	8323	-594	144	134	8007	93	
	4f ² + 5p4f	⁵ G ₄	9391	-3048	908	1102	8353	8845	-3330	801	1309	7624	-729	

TABLE VI. Comparison of the CI+all-order energies of Sn-like Ba^{6+} relative to the ground state calculated as two-valence-electron (2-val) and four-valence-electron (4-val) system (in cm^{-1}). Experimental results [20] are listed in column labeled “Expt.” The columns Δ_{2val} and Δ_{4val} give differences between 2-val and 4-val calculations and experiment. In the two-valence-electron calculation, the $5s$ shell is taken to be a core shell. The column labeled “Ave.” gives the average of the 4-val and 2-val calculations. In last column the difference of averaged results with experiment is presented.

Level	2-val	4-val	Expt.	Δ_{2val}	Δ_{4val}	Ave.	Δ_{Ave}
$5p^2\ ^3P_0$	0	0	0	0	0	0	0
$5p^2\ ^3P_1$	15477	15372	15507	30	135	15425	82
$5p^2\ ^3P_2$	21161	21422	21499	338	77	21291	208
$5p^2\ ^1D_2$	41888	42420	42514	626	94	42154	360
$5p^2\ ^1S_0$	61030	61602	61083	53	-519	61316	-233

ions of Cd-like isoelectronic sequence, La^{9+} , Ce^{10+} , and Pr^{11+} , and compared the results with the experimental values from [21–23]. We present the comparison of theoretical energies with experiment for all five consecutive ions of Cd-like isoelectronic sequence, Ba^{8+} [20], La^{9+} [21], Ce^{10+} [22], Pr^{11+} [23], and Nd^{12+} [24], in Table II. All energies are given relative to the $5s^2\ ^1S_0$ ground state in cm^{-1} . Actual (in cm^{-1}) and relative (in %) differences with experiment are given for all states. The states are listed in the same order for all five ions for the convenience of presentation. The actual order of states starts to change for Ce^{10+} . The fine-structure splittings of the $5s5p$ and $4f5s$ triplets are listed in the last four rows. Table II clearly illustrates the abrupt shift in the agreement with experiment between the first three and last two ions. It appears that all levels with the exception of the $5s5p\ ^1P_1$ suddenly shift by about $2000\ cm^{-1}$ for Pr^{11+} . We note that the $5s^2\ ^1S_0 - 5s5p\ ^1P_1$ is the only strong easily identifiable line from all of the states considered here. The

identification of other numerous ultraviolet (UV) lines is a very difficult task carried out in [21–23] using the Cowan code. It may be possible that change in the order of levels for Pr^{11+} resulted in some identification problem. Since our calculations are carried out in the same way for all ions, we find an abrupt $2000\ cm^{-1}$ shift in accuracy to be unlikely. Further measurements are needed to resolve this problem. We use the first (25%) approach to estimate the accuracy of our calculations for Sm^{14+} energies since $4f^2$ configuration is not present among measured low-lying levels of Ba^{8+} , and this reference ion cannot be used for Sm^{14+} .

The CI+all-order sensitivity coefficients q for Cd-like ions obtained as described in Sec. II are given in Table III. All energy and q values are given relative to the ground state in cm^{-1} . The CI+all-order energies and q coefficients are used to calculate enhancement factors $K = 2q/\omega$ given in the last row of the table. The enhancement factors are very large for all transitions from the $5s4f$ levels to the ground state for Sm^{14+} due to large q and small transition energies. The calculation of q for Ag-like ions [19] demonstrated that the effect of correlation is small for the cases where q are large, i.e., all cases of interest. Therefore, the uncertainties in large values of K will be dominated by the uncertainties in the transition energies, in particular where they exceed 2%–3%. Then, the relative uncertainty in K for $4f^2\ ^3H_4 - 5s4f$ transitions can be estimated as the relative uncertainty in the corresponding transition energy. We note that q values are positive for Nd^{12+} and negative for Sm^{14+} . This creates additional enhancements for α variation search if the relative transition frequencies in Nd^{12+}/Sm^{14+} are monitored.

The CI+all-order multipole reduced-matrix elements Z , transition rates A_r , and lifetimes τ in Cd-like Nd^{12+} and Sm^{14+} ions are given in Table IV. We use theoretical energies in transition rate and lifetime calculations. The numbers in brackets represent powers of 10. The strongest transition from the first excited levels of both ions is $M2$, leading to the

TABLE VII. Comparison of the CI+all-order energies of Sn-like Pr^{9+} and Nd^{10+} relative to the ground state calculated as two-valence-electron (2-val) and four-valence-electron (4-val) system (in cm^{-1}). The final numbers, which are the average of two calculations, are listed in the column labeled “Final.” Estimated absolute uncertainties of the respective values are given in columns “Unc.” in cm^{-1} . Wavelengths for transitions to the ground state and their uncertainties (in parentheses) are given in the last column in nm.

Ion	Term	J	2-val	Unc.	4-val	Unc.	Final	Unc.	λ
Pr^{9+}	$5p^2$	3P_0	0		0	0	0	0	
	$5p4f$	3G_3	20216	540	21895	450	21055	840	475(18)
	$5p4f$	3F_2	22772	430	24199	370	23485	710	426(13)
	$5p4f$	3F_3	25362	580	27002	570	26182	820	382(12)
	$5p4f$	3F_4	27536	560	29343	590	28440	900	352(11)
	$5p^2$	3P_1	28512	160	28436	320	28474	320	351.2(5)
	$5p^2$	3P_2	35653	240	36217	380	35935	380	278(2)
	$5p4f$	1F_3	53588	710	55220	710	54404	820	184(3)
Nd^{10+}	$4f^2$	3H_4	0	0	0	0	0	0	
	$5p4f$	5G_3	1564	1100	560	1300	1062	1300	
	$4f^2$	3H_5	3059	220	3058	210	3059	220	3270(220)
	$5p4f$	1D_2	5060	980	4040	1100	4550	1100	2200(430)
	$4f^2$	3H_6	6222	460	6219	430	6221	460	1610(110)
	$5p4f$	3F_3	7095	1200	6382	1320	6738	1320	1480(240)
	$4f^2 + 5p4f$	3F_2	7914	270	8007	240	7960	270	1260(40)
	$4f^2 + 5p4f$	5G_4	8353	940	7624	1070	7989	1070	1250(150)

extremely long lifetimes. The case of Nd^{12+} is very similar to Ag-like Nd^{13+} discussed in Ref. [19] but the wavelengths are further in UV. Next excited states in both ions live also very long, with 20 s and 8.5 s lifetimes for Nd^{12+} and Sm^{14+} , respectively.

IV. SN-LIKE IONS

The Sn-like ions, considered in this work, may be treated either as divalent systems with $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6 4d^{10} 5s^2$ core or systems with four valence electrons (then, the 5s electrons are in the valence field). We carry out both calculations to ensure that all dominant configurations are taken into account. We refer to the results of these calculations as 2-val and 4-val, respectively. We carried out the same calculations for the Ba^{6+} ion, which is the last ion in Sn isoelectronic sequence where experimental energies are available. Unfortunately, the experimental data for this ion are limited to the fine structure of the $5p^2$ configuration. The results of 2-val and 4-val calculations for Sn-like ions are summarized in Table V where we list the energies of Sn-like Ba^{6+} , Pr^{9+} , and Nd^{10+} ions relative to the ground state. Contributions from higher-order Coulomb correlation (difference of the CI+all-order and CI+MBPT calculations), estimated contributions of higher partial waves ($l > 6$), and Breit interaction are given separately in columns labeled ‘‘HO,’’ ‘‘Extrap,’’ and ‘‘Breit.’’ QED contribution is considered to be negligible for these states.

We find a technical complication in applying CI+all-order method to the Sn-like ions. Both the CI+MBPT and CI+all-order methods are based on the Brilloiun-Wigner variant of the MBPT, rather than the Rayleigh-Schrödinger to avoid nonsymmetric effective Hamiltonian and the problem of intruder states. In the Brilloiun-Wigner variant of MBPT, the effective Hamiltonian is symmetric and accidentally small denominators do not arise, but the many-body corrections to the Hamiltonian Σ_1 and Σ_2 become energy dependent. Solving the equation for H^{eff} we are able to find these energies. But

TABLE VIII. Transition energies, ω , and sensitivity coefficients q for Sn-like ions relative to the ground state evaluated in the CI+all-order approximation in cm^{-1} ; $K = 2q/\omega$ is the enhancement factor.

Ion	Term	J	ω	q	K
Pr^{9+}	$5p^2$	3P_0	0	0	
	$5p4f$	3G_3	20216	42721	4.2
	$5p4f$	3F_2	22772	42865	3.8
	$5p4f$	3F_3	25362	47076	3.7
	$5p4f$	3F_4	27536	37197	2.7
	$5p^2$	3P_1	28512	47483	3.3
Nd^{10+}	$4f^2$	3H_4	0		
	$5p4f$	5G_3	1564	-81052	-104
	$4f^2$	3H_5	3059	3113	2.0
	$5p4f$	1D_2	5060	-60350	-24
	$4f^2$	3H_6	6222	5930	1.9
	$5p4f$	3F_3	7095	-63285	-18
	$4f^2 + 5p4f$	3F_2	7914	-17809	-4.5
	$4f^2 + 5p4f$	5G_4	8353	-39672	-9.5

since we use the single-particle perturbation theory, a more simple and practical approach is to set this energy, $\tilde{\epsilon}$, to be the Dirac-Fock energy of the lowest orbital for the particular partial wave (see Refs. [26,28] for more details).

For all Cd-like calculations carried out in this work, this approach works perfectly fine. However, we find that the use of the lowest 5d energies, as $\tilde{\epsilon}$, is not appropriate for the 2-val calculations for the Sn-like ions. This is because the 5s state, which is treated as a core state in 2-val calculations, has small excitation energy, very close to the excitation energy of the 5d state. This leads to extremely small energy denominator in the expression for $\hat{\Sigma}$, e.g., $\epsilon_{5s} + \epsilon_{5d} - \epsilon_{5p} - \epsilon_{5p} \simeq 0$. This means that the sum of two single-electron energies $\epsilon_{5s} + \epsilon_{5d}$ is a poor approximation for the two-electron energies of low states of Sn-like ions which must enter the expression for $\hat{\Sigma}$. Therefore, we use the $5p_{1/2}$ energies for $\tilde{\epsilon}$ in the expressions for $\hat{\Sigma}$ operator for ns and nd states. The $4f_j$ energies are used for the nf states.

We have tested the sufficient completeness of the four-electron configuration space by carrying out three calculations with increasing number of configurations. The first run contained only double excitations into the valence space from a few main configurations. Two larger runs were selectively constructed by allowing extra excitations into the valence space from several hundreds most important configurations. Thus triple and quadrupole excitations from initial configurations were effectively included. The differences between the results of the first two runs were less than 350 cm^{-1} . The differences between the second and final largest runs with 23000 and 32000 configurations, respectively, were less than 10 cm^{-1} indicating sufficient saturation of the configuration space.

We provide a detailed comparison of 2-val and 4-val results with the experiment for Ba^{6+} [20] in Table VI. While we find a good agreement of both results with experiment, it is unclear whether 2-val or 4-val calculations provide better accuracy. The agreement with experiment is different for the four states. Most likely this is caused by the admixture of configurations that cannot be described as divalent $5s^2 n l n' l'$

TABLE IX. Absolute values of multipole reduced matrix elements obtained by CI+all-order two-valence-electrons (2-val) and four-valence-electrons (4-val) calculations in Sn-like Pr^{9+} ion (in a.u.).

	Transition	2-val	4-val
$M1$	$5p^2 \ ^3P_0 \rightarrow 5p^2 \ ^3P_1$	1.273	1.274
$M1$	$5p4f \ ^3F_2 \rightarrow 5p^2 \ ^3P_1$	0.323	0.359
$M1$	$5p4f \ ^3G_3 \rightarrow 5p4f \ ^3F_2$	0.320	0.312
$E2$	$5p^2 \ ^3P_0 \rightarrow 5p^2 \ ^3P_2$	1.901	1.864
$E2$	$5p^2 \ ^3P_0 \rightarrow 5p4f \ ^3F_2$	0.232	0.110
$E2$	$5p^2 \ ^3P_1 \rightarrow 5p4f \ ^1F_3$	0.623	0.577
$E2$	$5p4f \ ^3G_3 \rightarrow 5p^2 \ ^3P_1$	0.183	0.170
$E2$	$5p4f \ ^3F_3 \rightarrow 5p^2 \ ^3P_1$	1.133	1.071
$E2$	$5p4f \ ^3G_3 \rightarrow 5p4f \ ^3F_3$	0.117	0.089
$E2$	$5p4f \ ^3F_2 \rightarrow 5p4f \ ^3F_4$	0.662	0.686
$E2$	$5p4f \ ^3G_3 \rightarrow 5p4f \ ^1F_3$	2.109	2.071
$M3$	$5p^2 \ ^3P_1 \rightarrow 5p^2 \ ^3P_2$	13.369	14.162
$M3$	$5p^2 \ ^3P_0 \rightarrow 5p4f \ ^3G_3$	0.427	0.328
$M3$	$5p^2 \ ^3P_0 \rightarrow 5p4f \ ^3F_3$	4.906	5.246

states. It appears that the average of both calculations produces the results that are the most consistent with experiment for all states. Unfortunately, we have no comparison with experiment for the $5p4f$ and $4f^2$ configurations which are of interest for the present work.

The ions of interest in the Sn-like isoelectronic sequence are Pr^{9+} and Nd^{10+} , where the $5p^2$ and $5p4f$ or $5p4f$ and $4f^2$ levels become very close due to the $5p-4f$ level crossing. The case of Pr^{9+} is particularly interesting, since the several lowest metastable levels have transitions to the ground state in the optical range. The ground and first excited states of Nd^{10+} are extremely close and the resulting uncertainty is on the order of the transition energy. While our calculations place $4f^2$ to be the ground state, the higher-order corrections are particularly large in this case, almost three times that of the transition energy, which might lead to the placement of the $5p4f$ $J = 3$ as the ground state.

Determination of the uncertainties is difficult for these ions due to complete lack of data for comparison. We also observe strong cancellations between various large corrections. Therefore, adding 25% of all corrections in quadrature may significantly overestimate the uncertainties. We take the

average of the 25% estimate and the total sum of all corrections as an uncertainty for all levels and list these values. The uncertainties are independently evaluated for 2-val and 4-val calculations following this prescription. Comparison of the CI+all-order energies of Sn-like Pr^{9+} and Nd^{10+} relative to the ground state calculated as two-valence-electron and four-valence-electron system is given in Table VII. The final numbers, which are the average of two calculations, are listed in the column ‘‘Final.’’ Estimated uncertainties of all values are given in columns ‘‘Unc.’’ Wavelengths for transitions to the ground state are given in the last columns in nm. The sensitivity coefficients q for Sn-like Pr^{9+} and Nd^{10+} ions are given in Table VIII together with the corresponding CI+all-order transition energies and K enhancement factors.

Comparison of multipole matrix elements obtained from CI+all-order 2-val and 4-val calculations in Sn-like Pr^{9+} ion is given in Table IX. The differences are a few percent for most transitions, but significant for weak transitions, such as $E2$ $5p^2\ ^3P_0-5p4f\ ^3F_2$. It is expected since weak transitions are more sensitive to the admixtures of configurations which are omitted in the 2-val calculation.

TABLE X. CI+all-order multipole matrix elements Z (in a.u.), transition rates A_r (in s^{-1}), and lifetimes τ (in sec) in Sn-like Pr^{9+} and Nd^{10+} ions. Transition energies ΔE (in cm^{-1}) and wavelengths λ (in nm) are obtained from final energy values given by Table VII. The numbers in brackets represent powers of 10.

Ion	Term	Transition		ΔE	λ	Z	A_r	τ	
Pr^{9+}	$5p4f\ ^3G_3$	$5p^2\ ^3P_0$	$5p4f\ ^3G_3$	$M3$	21055	474.9	0.42712	2.001[−15]	4.997[+14]
		$5p^2\ ^3P_0$	$5p4f\ ^3F_2$	$E2$	23485	425.8	0.23230	8.635[−03]	51.8
	$5p4f\ ^3F_2$	$5p4f\ ^3G_3$	$5p4f\ ^3F_2$	$M1$	2430	4115	0.31981	7.917[−03]	
		$5p4f\ ^3F_2$	$5p4f\ ^3F_3$	$M1$	2697	3708	1.67447	2.120[−01]	4.718
	$5p4f\ ^3F_3$	$5p4f\ ^3G_3$	$5p4f\ ^3F_4$	$M1$	7385	1354	1.89256	4.324[+00]	0.227
	$5p4f\ ^3F_4$	$5p4f\ ^3F_3$	$5p4f\ ^3F_4$	$M1$	2258	4429	1.46389	7.394[−02]	
		$5p^2\ ^3P_1$	$5p^2\ ^3P_1$	$M1$	28474	351.2	1.27262	3.362[+02]	2.975[−3]
	$5p^2\ ^3P_2$	$5p^2\ ^3P_0$	$5p^2\ ^3P_2$	$E2$	35935	278.3	1.90140	4.852[+00]	0.0838
		$5p4f\ ^3G_3$	$5p^2\ ^3P_2$	$M1$	14880	672.0	0.20488	7.461[−01]	
	$5p4f\ ^1F_3$	$5p4f\ ^3F_2$	$5p^2\ ^3P_2$	$E2$	12450	803.2	0.60441	2.448[−03]	
		$5p4f\ ^3F_3$	$5p^2\ ^3P_2$	$M1$	9753	1025	0.90901	4.135[+00]	
		$5p^2\ ^3P_1$	$5p^2\ ^3P_2$	$M1$	7461	1340	0.99055	2.198[+00]	
		$5p4f\ ^3F_2$	$5p4f\ ^1F_3$	$M1$	30919	323.4	1.02292	1.192[+02]	7.382[−3]
		$5p4f\ ^3G_3$	$5p4f\ ^1F_3$	$E2$	33349	299.9	2.10930	2.936[+00]	
		$5p4f\ ^3F_4$	$5p4f\ ^1F_3$	$M1$	25964	385.1	0.25958	4.545[+00]	
	Nd^{10+}	$5p4f\ ^5G_3$	$5p^2\ ^3P_2$	$5p4f\ ^1F_3$	$M1$	18469	541.4	0.60127	8.776[+00]
$4f^2\ ^3H_4$			$5p4f\ ^5G_3$	$M1$	1062	9416	0.06522	1.963[−05]	5.094[+04]
$4f^2\ ^3H_5$		$4f^2\ ^3H_4$	$4f^2\ ^3H_5$	$M1$	3059	3269	3.21593	7.259[−01]	1.378
		$5p4f\ ^1D_2$	$5p4f\ ^5G_3$	$5p4f\ ^1D_2$	$M1$	3488	2867	0.41514	3.945[−02]
$4f^2\ ^3H_6$		$4f^2\ ^3H_4$	$5p4f\ ^1D_2$	$E2$	4550	2198	0.66642	1.940[−05]	
		$4f^2\ ^3H_5$	$4f^2\ ^3H_6$	$M1$	3162	3163	3.26836	7.007[−01]	1.427
$5p4f\ ^3F_3$		$5p4f\ ^1D_2$	$5p4f\ ^3F_3$	$M1$	2188	4570	1.94864	1.533[−01]	3.916
		$5p4f\ ^5G_3$	$5p4f\ ^3F_3$	$M1$	5676	1762	0.36934	9.612[−02]	
$4f^2 + 5p4f\ ^3F_2$		$4f^2\ ^3H_4$	$5p4f\ ^3F_3$	$M1$	6738	1484	0.07115	5.967[−03]	
		$5p4f\ ^1D_2$	$4f^2 + 5p4f\ ^3F_2$	$M1$	3410	2933	0.29565	1.870[−02]	43.92
		$5p4f\ ^5G_3$	$4f^2 + 5p4f\ ^3F_2$	$M1$	6898	1450	0.04406	3.437[−03]	
		$4f^2\ ^3H_4$	$4f^2 + 5p4f\ ^3F_2$	$E2$	7960	1256	0.93855	6.305[−04]	
$4f^2 + 5p4f\ ^5G_4$		$5p4f\ ^5G_3$	$4f^2 + 5p4f\ ^5G_4$	$M1$	6927	1444	1.57004	2.456[+00]	0.365
		$4f^2\ ^3H_4$	$4f^2 + 5p4f\ ^5G_4$	$M1$	7989	1252	0.38552	2.271[−01]	
		$4f^2\ ^3H_5$	$4f^2 + 5p4f\ ^5G_4$	$M1$	4930	2028	0.36808	4.865[−02]	
		$5p4f\ ^3F_3$	$4f^2 + 5p4f\ ^5G_4$	$M1$	1251	7994	1.39879	1.148[−02]	

The CI+all-order multipole matrix elements Z , transition rates A_r , and lifetimes τ in Sn-like Pr^{9+} and Nd^{10+} ions are presented in Table X. Energies are final results presented in Table VII. The numbers in brackets represent powers of 10. We highlight the case of Pr^{9+} where the lowest metastable state, $5p4f^3G_3$, has a very long lifetime with $M3$ 495 nm transition to the ground state being in the optical range. The next two levels, $5p4f^3F_2$ and $5p4f^3F_3$, also have optical transitions to the ground state and are metastable with 59 s and 5.3 s lifetimes. A relatively strong $M1$ transition to the ground state from $5p^2^3P_1$ level at 351 nm may be potentially used for cooling and probing. Our Nd^{10+} transition property calculations assume that $4f^2 J = 4$ level is the ground state. While several low levels of Nd^{10+} are long lived, the corresponding transitions are all far in the infrared.

V. CONCLUSION

We carried out detailed high-precision study of Cd-like Nd^{12+} , Sm^{14+} and Sn-like Pr^{9+} , Nd^{10+} atomic properties using

a hybrid approach that combines configuration interaction and a linearized coupled-cluster method. These highly charged ions are of interest for future experimental studies aimed at the development of ultraprecise atomic clocks and search for α variation. Energies, transition wavelengths, electric- and magnetic-multipole reduced-matrix elements, lifetimes, and the sensitivity coefficients to α variation, q and K , were calculated. Several methods to evaluate uncertainties of the results were developed.

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