

## Calculation of atomic properties of superheavy elements $Z = 110$ – $112$ and their ions

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We calculate the spectra, electric dipole transition rates, and isotope shifts of the superheavy elements Ds ( $Z = 110$ ), Rg ( $Z = 111$ ), and Cn ( $Z = 112$ ) and their ions. These calculations were performed using a recently developed, efficient version of the *ab initio* configuration-interaction combined with perturbation theory to treat distant effects. The successive ionization potentials of the three elements are also calculated and compared to lighter analogous elements.

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### I. INTRODUCTION

The discovery and study of superheavy elements (SHEs, where  $Z > 103$ ) have been of great interest both experimentally and theoretically to physicists for the past 50 years. Their large nuclear charge is predicted to result in exotic atomic properties which are not observed in other elements and break well established trends in the periodic table. While SHEs up to  $Z = 118$  have been experimentally synthesized and recognized, their low production rates and short half-lives have made the study of chemical and physical properties difficult (see reviews [1–3]). As such, there are no experimental data on their spectra though there has been experimental success in measuring the ionization potentials and singly excited states in No and Lr which lie just below the SHEs [4–6]. Therefore, until further development of experimental techniques, the study of electron properties of SHEs must be made in the theoretical domain using many-body approaches. Such theoretical calculations will not only help further the understanding exotic properties SHEs, they are also predictive and will aid both future experimental measurements and the search for metastable isotopes in astronomical data. While there are currently no direct observations of these metastable isotopes or the island of stability in astronomical data, indirect observations and theoretical predictions support their existence [7].

Most SHEs in the region  $Z = 103$  to  $Z = 118$  have open shells, with up to ten electrons in these shells. Theoretical study of such systems is difficult due to the fast increase of the number of possible configurations with the number of electrons. There are few powerful methods of many-body relativistic calculations which work very well for atoms with relatively simple electron structure, having one to four electrons above closed shells. These were used in a number of studies of SHEs which fell into this category (see, e.g., [8,9]). The use of these methods in systems with more than four external electrons is problematic due to the high demand for computer power. Also, techniques which extrapolate results of lighter elements are insufficient for treating SHEs due to the large relativistic effects which result in exotic properties which do not exist in lighter elements. An efficient *ab initio*

method capable of calculating the spectroscopic properties of these elements has been developed in [10] which combines configuration interaction (CI) and perturbation theory (PT) referred to as the CIPT method.

The CIPT method has been used for the open- $6d$ -shell SHEs Db ( $Z = 105$ ) [11], Sg ( $Z = 106$ ), Bh ( $Z = 107$ ), Hs ( $Z = 108$ ), and Mt ( $Z = 109$ ) [12] along with the closed-shell noble SHE Og ( $Z = 118$ ) [13]. This method has also been used to accurately calculate the low-lying states of Ta [11] and Rn [13] (lighter elemental analogs of Db and Og respectively) when compared to available experimental data. This paper will focus on the heaviest SHE “metals” in groups 10, 11, and 12, specifically darmstadtium (Ds,  $Z = 110$ ), roentgenium (Rg,  $Z = 111$ ), and copernicium (Cn,  $Z = 112$ ). In particular, these SHEs are of interest as their proton number lies close to the expected magic number for stability,  $Z = 114$ , and therefore the existence of long-lived meta-stable isotopes is promising [1]. The expected magic numbers of neutrons for these meta-stable nuclei has been calculated to be  $N = 184$ . The search for these meta-stable SHEs and the “island of stability” has been at the frontier of nuclear physics for decades. These neutron rich nuclei cannot be produced in laboratory conditions, however it has been suggested that the neutron flux, which occurs in cosmological events, could create these metastable nuclei [14–17]. A promising method for detecting traces of these isotopes in astrophysical data using calculated isotope shifts and experimental data from unstable, neutron deficient isotopes in laboratories was presented in Ref. [18]. To accommodate searches, in this work we also present the isotope shifts of the neutral atoms and ions Ds I, II, III, and Rg I, II for available optical  $E1$  transitions. While some states of Rg I and Cn I have been calculated previously (see Secs. III and IV) there has not been significant treatment of the ionic states of these elements or their isotope shifts.

The ground states for the three elements have been found to be  $[\text{Rn}]6d^n7s^2$  where  $n = 8, 9, 10$  for Ds, Rg, and Cn respectively. The Cn atom has a relatively simple electron structure with completely closed shells in its ground state. Therefore, theoretical predictions of its spectra do exist; they were calculated using *ab initio* techniques such as multiconfigurational Dirac-Fock (MCDF) [19], relativistic

pseudopotentials (RPPs) [20], CI + many-body perturbation theory (MBPT) [21], and relativistic coupled cluster (RCC) [22] methods. Similarly for Rg, which is one electron short of a closed  $6d$  shell, the RPP method has been used to calculate some states in the excitation spectrum with which we can compare our results.

This paper progresses as follows, in Sec. II we give a brief overview of the CIPT method and how it is implemented for SHE. In Secs. III and IV we present the calculated low-lying excitation spectrum of Ds I, II, III, and Rg I, II, and Cn I, II, III. In Secs. V and VI we present the optical  $E1$  transitions and corresponding isotope shifts, and the successive ionization potentials of Ds, Rg, and Cn respectively.

## II. CIPT METHOD

As mentioned above, a configuration-interaction approach to calculate the spectra of atoms with unfilled shells has been developed [10] and has been used to calculate the spectra, IPs, and transition rates in SHEs  $Z = 102$ ,  $105$ – $109$ , and  $Z = 118$  and their respective lighter elemental analogs [10–13]. Recently the efficiency of this method has been improved upon with only a small additional cost of accuracy [23]. In this work we will give a brief overview of the method.

To generate the single-electron basis states a  $V^{N_e-1}$  (where  $N_e$  is the total number of electrons) Hartree-Fock (HF) approximation is used. In this approximation, the HF calculations are performed for the charged open-shell ion with one electron removed from the atom or ion of interest [24,25]. In most of the cases an external  $s$  electron is removed. However, in some cases, for example the calculations of even states of Au I and Hg II, better accuracy is achieved if a  $5d$  electron is removed. The multielectron basis sets are then generated using a  $B$ -splines technique with 40  $B$ -spline states in each partial wave of order 9 in a box of radius  $40a_B$  (where  $a_B$  is the Bohr radius) with partial waves up to  $l_{\max} = 4$ . The single determinant many-electron basis states  $|i\rangle = \Phi_i(r_1, \dots, r_{N_e})$  for the CI calculations are generated by making all single and double electron excitations from reference configurations.

The CI wave function  $|\Psi\rangle$  is written as an expansion over single-determinant many-electron states from two distinct sets of the many-electron basis states  $|i\rangle$ ,

$$|\Psi\rangle = \sum_{i=1}^{N_{\text{Eff}}} c_i |i\rangle + \sum_{i=N_{\text{Eff}}+1}^{N_{\text{total}}} c_i |i\rangle. \quad (1)$$

The first summation in Eq. (1) represents a small set of low-energy wave functions which give a good approximation to the state ( $i \leq N_{\text{Eff}}$ , where  $N_{\text{Eff}}$  is the number of wave functions in the low-energy set). The second summation in Eq. (1) is a large set of high-energy wave functions which are corrections to the state. The CI matrix is constructed by ordering the basis states  $|i\rangle$  according to their energy and dividing them into two sets of low-energy and high-energy states. The CI matrix is simplified by neglecting all off diagonal matrix elements of the CI matrix between the terms in the high-energy set,  $\langle i|H^{\text{CI}}|j\rangle = 0$  for  $|i\rangle, |j\rangle > N_{\text{Eff}}$ . This truncation of the matrix significantly reduces the previous large diagonalization problem to a simplified CI diagonalization problem of size  $N_{\text{Eff}}$ . This smaller matrix of size  $N_{\text{Eff}} \times N_{\text{Eff}}$  is referred to as the

effective CI matrix,

$$(H^{\text{CI}} - EI)X = 0, \quad (2)$$

where  $I$  is unit matrix, and the vector  $X = \{c_1, \dots, c_{N_{\text{Eff}}}\}$ . The high-energy basis states  $i > N_{\text{Eff}}$  are included by modifying the matrix elements of the effective CI matrix. Specifically, the matrix elements of the effective CI matrix are modified to include perturbative contributions from the high-energy states,

$$\langle i|H^{\text{CI}}|j\rangle \rightarrow \langle i|H^{\text{CI}}|j\rangle + \sum_k \frac{\langle i|H^{\text{CI}}|k\rangle \langle k|H^{\text{CI}}|j\rangle}{E - E_k}. \quad (3)$$

where  $i, j \leq N_{\text{Eff}}$ ,  $k > N_{\text{Eff}}$ ,  $E_k = \langle k|H^{\text{CI}}|k\rangle$ , and  $E$  is the energy of the state of interest. As this energy is not known *a priori*, iterations of the second summation must be performed until there is a convergence in  $E$ . When this convergence is achieved, the energy is an exact solution to the truncated CI matrix. This is known as the CIPT method.

The Breit interaction [26,27] and quantum electrodynamic (QED) radiative corrections (Ueling potential and electric and magnetic form factors) [28] are included in the calculations as described in our earlier works (see, e.g., [29]). As both the Breit and QED radiative corrections scale with nuclear charge  $Z$  faster than the first power [29], their contribution to the energy levels of SHE is non-negligible. This radiative potential method reproduces accurate QED calculations in heavy single electron ions to 0.1–0.5% in high  $s$  states, 1–3% in high  $p_{1/2}$  states, and 1–9% in high  $p_{3/2}$  states (see Table I in Ref. [28]). In many-electron atoms QED corrections are dominated by the  $s_{1/2}$  orbitals and many-body effects due to interaction of the other electrons with the  $s_{1/2}$  orbitals. Therefore, this radiative potential approach is sufficient for the accuracy of our calculations. Also, it has been checked earlier that the results for QED corrections using our approach in other atoms practically coincide with the results of Shabeav *et al.* in Ref. [30]. For each level we calculate the Landé  $g$  factor for comparison with experimental  $g$  factors in lighter elements. To label the levels in the SHE spectra for reference, we compare the SHE states to similar states in lighter analogs with similar  $g$  factors, and if available, adopt that notation for the SHE state. However it should be noted that  $LS$  notation is not, in general, appropriate for labeling SHE states. This is due to very large spin-orbit interaction in SHEs (so the eigenvectors will look strongly mixed in  $LS$  notation). We only use  $LS$  notations for comparison with lighter elements. If analogous states of the lighter element are not available with  $LS$  notation we label the  $n$ th sequential state of total angular momentum  $J$  and parity by  $n_J^{\text{parity}}$ . We use the same notation for presenting states of lighter elements when  $LS$  notation is not available. For the SHE energy levels we present the configuration weight of the major configuration where it is strongly mixed (<70%). For all the other levels the configuration presented is dominant.

## III. DS AND RG

Both elements darmstadtium and roentgenium were synthesized in 1994 [31,32] and officially named and recognized in 2001 [33]. Early theoretical calculations of their ground states show that they are anomalous in each of their groups.

TABLE I. Comparison of CIPT energy-level calculations for neutral Pt I, II, and Pd III with experimental values. Low-lying even and odd states for Ds I, Ds II, and Ds III calculated using the CIPT energy. Experimental energies and CIPT energies are given by  $E_E$  and  $E_T$  respectively. Where available, the experimental Landé  $g$  factors  $g_E$  are provided for comparison. The discrepancy between the experimental and CIPT energies is given by  $\Delta = E_E - E_T$ . The configuration weights for strongly mixed states of Ds I, II, and III are also presented. For other states the leading configuration weight is  $>70\%$ .

State	Experimental [35]		CIPT		$\Delta$		CIPT			
	$E_E$ (cm $^{-1}$ )	$g_E$	$E_T$ (cm $^{-1}$ )	$g_T$			State	$E_T$	$g_T$	
Pt I										
Even states										
$5d^9 6s$	$^3D_3$	0	0	1.33		$6d^8 7s^2$	$^3F_4$	0	1.23	
$5d^9 6s$	$^3D_2$	776	1.01	728	1.07	48	$^3P_2$	4146	1.12	
$5d^8 6s^2$	$^3F_4$	824	1.25	1289	1.24	-465	0	14 541	0.00	
$5d^{10}$	$^1S_0$	6140		5148	0.00	992	$^3F_3$	16 499	1.08	
$5d^9 6s$	$^3D_1$	10 132		8889	0.50	1243	$^3P_1$	23 322	1.50	
Odd states										
$5d^8 6s 6p$	$^5D_4^o$	30 157	1.46	31 390	1.46	-1233	$6d^7 7s^2 7p$	$1_4^o$	21 812	1.34
$5d^9 6p$	$1_2^o$	32 620	1.39	31 652	1.38	968	$6d^7 7s^2 7p$	$1_5^o$	24 958	1.23
$5d^8 6s 6p$	$1_5^o$	33 681	1.32	34 662	1.31	-981	$6d^7 7s^2 7p$	$1_1^o$	26 779	1.44
$5d^9 6p$	$1_3^o$	34 122	1.21	33 141	1.13	981	$6d^7 7s^2 7p$	$1_2^o$	28 550	1.07
$5d^8 6s 6p$	$2_3^o$	35 322	1.33	36 479	1.36	-1157	$6d^7 7s^2 7p$	$2_2^o$	30 383	1.34
$5d^8 6s 6p$	$2_4^o$	36 296		36 394	1.25	-98	$6d^7 7s^2 7p$	$1_3^o$	32 645	1.16
$5d^8 6s 6p$	$^5G_6$	36 782	1.33	37 603	1.33	-821	$6d^7 7s^2 7p$	$2_3^o$	36 404	1.25
$5d^9 6p$	$2_1^o$	36 845	1.09	36 761	1.16	84	$6d^7 7s^2 7p$	$2_4^o$	34 919	1.38
$5d^9 6p$	$1_2^o$	37 342	1.15	36 889	1.14	453	$6d^7 7s^2 7p$	$3_4^o$	39 814	1.15
$5d^9 6p$	$3_4^o$	37 591	1.25	37 615	1.17	-24	$6d^7 7s^2 7p$	(59%) $2_5^o$	40 173	1.27
$5d^9 6p$	$3_3^o$	37 769	1.17	37 218	1.24	551	$6d^7 7s^2 7p$	$1_0^o$	40 668	0.00
$5d^8 6s 6p$	$^5F_5^o$	38 536	1.30	39 451	1.31	-915	$6d^7 7s^2 7p$	$3_2^o$	42 632	1.29
$5d^8 6s 6p$	$2_2^o$	38 816	0.88	39 275	0.76	-459	$6d^7 7s^2 7p$	(69%) $3_5^o$	42 682	1.22
$5d^8 6s 6p$	$4_4^o$	40 194.2	1.21	41 329	1.23	-1 135	$6d^7 7s^2 7p$	(53%) $3_3^o$	42 722	1.26
$5d^8 6s 6p$	$3_2^o$	40 516.3	1.38	41 968	1.23	-1 452	$6d^7 7s^2 7p$	$1_6$	42 322	1.28
$5d^8 6s 6p$	$4_2^o$	40 787.9	1.20	42 262	1.35	-1 474	$6d^7 7s^2 7p$	$2_1^o$	42 828	0.78
$5d^9 6p$	$2_0^o$	40 873.5		41 467	0.00	-594	$6d^7 7s^2 7p$	$4_2^o$	42 900	1.10
$5d^8 6s 6p$	$4_3^o$	40 970.1	1.12	41 991	1.09	-1 021	$6d^7 7s^2 7p$	(69%) $4_4^o$	43 915	1.18
$5d^8 6s 6p$	$3_1^o$	41 802.7	0.92	41 916	0.82	-113	$6d^7 7s^2 7p$	$4_3^o$	44 974	1.23
$5d^8 6s 6p$	$5_3^o$	42 660.2	1.19	44 087	1.14	-1 427	$6d^8 7s 7p$	(63%) $5_2^o$	45 149	1.29
$5d^8 6s 6p$	$4_1^o$	43 187.8	1.39	44 300	1.31	-1 112	$6d^7 7s^2 7p$	$2_0^o$	46 009	0.00
Pt II										
Even states										
$5d^9$	$^2D_{5/2}$	0.0		0	1.20		$6d^7 7s^2$	$^4F_{9/2}$	0	1.27
$5d^8 6s$	$^4F_{9/2}$	4786.6		4653	1.33	134	$6d^7 7s^2$	$^4F_{3/2}$	4464	1.20
$5d^9$	$^2D_{3/2}$	8419.9		8031	0.79	389	$6d^7 7s^2$	$^4F_{5/2}$	8484	1.21
$5d^8 6s$	$^4F_{7/2}$	9356.2		9166	1.20	190	$6d^7 7s^2$	$^4F_{7/2}$	15 407	1.20
$5d^8 6s$	$^4P_{1/2}$	21 718		22 886	2.57	-1168	$6d^7 7s^2$	$1_{1/2}$	21 178	1.37
							$6d^7 7s^2$	$1_{11/2}$	28 183	1.09
Odd states										
$5d^8 6p$	$^4D_{7/2}^o$	51 408		52 054	1.35	-646	$6d^6 7s^2 7p$	$1_{7/2}^o$	37 951	1.43
$5d^8 6p$	$^4G_{9/2}^o$	53 876		54 046	1.18	-170	$6d^6 7s^2 7p$	(62%) $1_{3/2}^o$	38 415	1.48
$5d^8 6p$	$^4D_{3/2}^o$	56 588		58 285	1.26	-1697	$6d^7 7s 7p$	$1_{9/2}^o$	39 010	1.42
$5d^8 6p$	$^4G_{5/2}^o$	57 018		58 198	1.16	-1180	$6d^6 7s^2 7p$	(67%) $1_{5/2}^o$	40 654	1.25
							$6d^6 7s^2 7p$	$2_{9/2}^o$	41 911	1.28
Ds II										

TABLE I. (Continued.)

State	Experimental [35]		CIPT		$\Delta$	State	CIPT		
	$E_E$ (cm <sup>-1</sup> )	$g_E$	$E_T$ (cm <sup>-1</sup> )	$g_T$			$E_T$	$g_T$	
	Pd III					Ds III			
Even states									
$4d^8$ $^3F_4$	0		0	1.25		$6d^67s^2$ (53%)	$1_2$	0	1.37
$4d^8$ $^3F_3$	3229		3173	1.08	56	$6d^77s$	$^5F_5$	1412	1.35
$4d^8$ $^3F_2$	4686		4695	0.70	-9	$6d^67s^2$	$^5F_4$	1675	1.32
$4d^8$ $^3P_1$	13 469		14 787	1.50	-1318	$6d^67s^2$	$1_0$	12 795	0.00
$4d^8$ $^3P_0$	13 698		15 212	0.00	-1514	$6d^77s$ (64%)	$^5F_1$	13 279	1.15
$4d^75s$ $^5F_5$	52 916		51 230	1.40	1686	$6d^77s$	$^5F_3$	13 376	1.38
Odd states									
$4d^75p$ $^5D_4^o$	104 418.86		101 793	1.41	-2626	$6d^67s7p$	$1_4^o$	45 317	1.54
						$6d^67s7p$ (54%)	$1_2^o$	48 521	1.71
						$6d^67s7p$	$1_5^o$	51 498	1.41

Consider both of the lighter elemental analogs Pt and Au which have ground states  $5d^96s$  and  $5d^{10}6s$  respectively. The large relativistic effects in Ds and Rg directly stabilize the  $7s$  orbital and indirectly destabilize the  $6d$  orbital resulting in ground states of  $6d^87s^2$  and  $6d^97s^2$  [34] respectively. The ground state of Ds and Rg both follow the same trend of the other open  $6d$ -shell elements which have closed  $7s$ -shell ground states. Using the CIPT method described in Sec. II we calculate the low-lying excitation spectrum of both Ds I, II, III in Table I and Rg I, II in Table III. To gauge the accuracy of the atomic calculations we also calculated the energy levels of Pt I, Pt II, and Pd III for comparison with available experimental results in Table I.

For Pt I and Pt II the even states are calculated using the reference states  $5d^{n-1}6s$ ,  $5d^{n-2}6s^2$ , and  $5d^n$  and odd states are calculated with reference states  $5d^{n-2}6s6p$ ,  $5d^{n-3}6s^26p$ , and  $5d^{n-1}6p$  where  $n = 10$  and  $9$  for the neutral atom and ion respectively. The CI matrix is populated with all single and double excitations of these reference states. Similarly for the calculations of Pd III we used reference states  $4d^75s$ ,  $4d^66s^2$ , and  $4d^8$  for the even states and  $4d^85s5p$ ,  $4d^75s^25p$ , and  $4d^95p$  for odd states. The spectrum of Pd III is calculated for comparison as there are no available experimental data for Pt III.

From Table I we see that there is good agreement between experimental results aggregated in Ref. [35] and the CIPT calculations of Pt I, II, and Pd III. While not as consistently accurate as the calculations of Ta in Ref. [11] which had an accuracy of  $|\Delta| \approx 500$  cm<sup>-1</sup>, for both the odd- and even-parity states of Pt I and Pt II there is agreement to within  $|\Delta| \approx 1500$  cm<sup>-1</sup> for low-lying states. For higher states the absolute energy difference between experimental and theoretical results is larger but the relative difference is only  $\sim 2\%$ . We expect this level of accuracy to be similar for the calculations of neutral Ds and the respective ions using the CIPT method.

To calculate the excitation spectrum of Ds I, II, and III reference configurations  $6d^{n-1}7s$ ,  $6d^{n-2}7s^2$ , and  $6d^n$  (even states) and  $6d^{n-2}7s7p$ ,  $6d^{n-3}7s^27p$ , and  $6d^{n-1}7p$  (odd states) are used to populate the effective CI matrix for  $n = 10, 9$ , and  $8$  respectively. Comparing the spectra of neutral Ds and its

ions with the spectra of lighter elemental analog we see that while they are in the same elemental group in the periodic table, there are some stark differences between their spectra. As previously mentioned, the ground state of Ds I follows the SHE trend of a closed  $7s^2$  shell unlike Pt I. The relativistic contraction of the  $7s$  shell and consequent destabilization of the  $6d$  shell in the SHE spectra results in a majority of odd-parity states from the excitation of the  $6d$  electron to the  $7p$  shell. Comparatively, the lighter analog spectrum of odd states is dominated by excitations of the  $6s$  electron to the  $6p$  shell. This lowers the odd-parity spectrum of Ds I with the first odd-parity state  $1_4^o$  at  $21\,812$  cm<sup>-1</sup> compared to the lowest state  $^5D_4^o$  at  $30\,157$  cm<sup>-1</sup>. This can also be seen in the odd-parity spectrum of Ds II when compared to Pt II. In Pt II the first odd-parity state is located far outside the optical region at  $51\,408$  cm<sup>-1</sup> while there are at least five odd-parity states in the Ds II spectrum which could potentially be detected through optical transitions to the ground state. This is similar to what was found when comparing the lighter open  $6d$ -shell elements to their respectively lighter analogs in Refs. [11,12]. The electric dipole ( $E1$ ) amplitudes and transition rates of these optically accessible states are calculated in Sec. V.

The excitation spectrum of Rg I and Rg II was calculated using the CIPT method and the results are presented in Table III. The CIPT calculation of Rg was very similar to Ds. The reference configurations used to populate the CI matrix are  $6d^{n-1}7s$ ,  $6d^{n-2}7s^2$  (even states), and  $6d^{n-2}7s7p$ ,  $6d^{n-3}7s^27p$ , and  $6d^{n-1}7p$  (odd states) where  $n = 11$  and  $10$  for Rg I and Rg II respectively. As for the Pt/Pd and Ds calculations both the neutral and first ion spectrum of Au were calculated to determine the accuracy of the Rg calculations. The Au calculations used similar appropriate reference configurations to Rg and are presented in Table II with experimental results for comparison. We see that the accuracy of the Au calculations is similar to that for Pt and Pd ( $|\Delta| \approx 1500$  cm<sup>-1</sup>). We expect a similar level of accuracy for the CIPT calculations of Rg I and Rg II which are presented in Table III.

The CIPT method results of Rg I and Rg II agree with the early calculations of Ref. [34] which found Rg I has a



TABLE II. Comparison of CIPT energy-level calculations,  $E_T$ , and experimental energy levels,  $E_E$ , results for Au and Au II. Where available, the experimental Landé  $g$  factors,  $g_E$ , are given along with calculated  $g$  factors,  $g_T$ . The difference between the experimental and theoretical energies is also presented,  $\Delta = E_E - E_T$ .

State	$E_E$ [35] ( $\text{cm}^{-1}$ )	$g_E$	$E_T$ ( $\text{cm}^{-1}$ )	$g_T$ ( $\text{cm}^{-1}$ )	$\Delta$ ( $\text{cm}^{-1}$ )
Au I					
Even states					
$5d^{10}6s$ $^2S_{1/2}$	0	1.997	0	2.00	
$5d^96s^2$ $^2D_{5/2}$	9161.77	1.192	10 902	1.20	-1740
$5d^96s^2$ $^2D_{3/2}$	21 435.191	0.804	22 361	0.80	-926
Odd states					
$5d^{10}6p$ $^2P_{1/2}^o$	37 358.991	0.661	38 722	0.67	-1363
$5d^{10}6p$ $^2P_{3/2}^o$	41 174.613	1.334	42 648	1.33	-1473
Au II					
Even states					
$5d^{10}$ $^1S_0$	0		0	0	
$5d^96s$ $^3D_3$	15 039.572		15 887	1.33	-847
$5d^96s$ $^3D_2$	17 640.616		18 551	1.20	-910
$5d^96s$ $^3D_1$	27 765.758		27 854	0.50	-88
Odd states					
$5d^96p$ $1_2^o$	63 053.318	1.45	64 964	1.39	-1910

ground state of  $6d^97s^2$  ( $^2D_{5/2}$ ). As seen in Ds, the odd-parity energies of Rg I have been shifted lower in the spectrum when compared to Au I. In Au I there are at most two viable optical  $E1$  transitions from the ground state whereas in Rg I there are five promising transitions. In Au II there are no optically accessible states, where there two potential states in Rg II.

Unlike Ds, some excitation levels and ionization potentials of Rg I have been previously calculated in Ref. [20] using a pseudopotential method and in Ref. [34] using a relativistic coupled cluster method. These values are included for comparison in Table III. While our CIPT calculations are within  $2000 \text{ cm}^{-1}$  of these calculations, they are always lower. While there has been calculation of odd-parity states of Rg I in Ref. [20] they only consider the excitation  $7s \rightarrow 7p$  above a closed- $6d$  shell. The  $E1$  transitions of Rg I and Rg II along with the corresponding isotope shifts have been included in Sec. V.

#### IV. CN

Copernicium (Cn) was first synthesized in 1996 [36] in Darmstadt, Germany. In particular the isotope  $^{277}\text{Cn}$  was synthesized which has a half-life of 200 ps which is too short for chemical study. Compared to Ds and Rg, there has been considerably more theoretical and experimental study on Cn where chemical properties such as its interaction with gold have been investigated [37]. This is primarily due to the closed- $6d$  shell in the ground state and some excited states. Calculations for such states can be done with many different methods. There has been significant theoretical study on the excitation spectrum compared to the lighter SHEs. Many-body techniques such as relativistic coupled cluster

TABLE III. Low-lying even and odd states for Rg I and Rg II calculated using the CIPT energy. The theoretical CIPT energies are given by  $E_{\text{CIPT}}$  and the Landé  $g$  factors are given by  $g_{\text{CIPT}}$ . Where available, previously calculated states using a pseudopotential method in Ref. [20] are given by  $E_{\text{PP}}$  for comparison. The configuration weights for the strongly mixed states are also presented.

State ( $\text{cm}^{-1}$ )	$E_{\text{CIPT}}$	$g_{\text{CIPT}}$ ( $\text{cm}^{-1}$ )	$E_{\text{RCC}}$ [34] ( $\text{cm}^{-1}$ )	$E_{\text{PP}}$ [20]
Rg I				
Even states				
$6d^97s^2$ $^2D_{5/2}$	0	1.20		
$6d^97s^2$ $^2D_{3/2}$	19 174	0.80	21 670	20 250
$6d^{10}7s$ $^2S_{1/2}$	22 428	2.00	23 820	24 760
Odd states				
$6d^87s^27p$ $1_{7/2}^o$	28 224	1.32		
$6d^87s^27p$ $1_{9/2}^o$	31 795	1.17		
$6d^87s^27p$ $1_{3/2}^o$	32 677	1.13		
$6d^87s^27p$ $1_{5/2}^o$	34 398	1.07		
$6d^97s7p$ $^4P_{5/2}^o$	42 709	1.46		
$6d^87s^27p$ $1_{1/2}^o$	44 292	0.72		
$6d^97s7p$ (67%) $^4F_{7/2}^o$	46 619	1.22		
$6d^87s^27p$ $3_{5/2}^o$	47 517	1.13		
$6d^97s7p$ (56%) $^4P_{3/2}^o$	48 547	1.40		
Rg II				
Even states				
$6d^87s^2$ $^3F_4$	0	1.23		
$6d^87s^2$ $1_2$	3786	1.11		
$6d^97s$ $^3D_3$	12 255	1.33	13 950	16 720
$6d^87s^2$ $1_0$	15 754	0.00		
$6d^87s^2$ $^3P_1$	28 105	1.50		
Odd states				
$6d^77s^27p$ $1_4^o$	42 047	1.32		
$6d^87s7p$ $2_4^o$	44 863	1.41		
$6d^77s^27p$ $1_1^o$	45 219	1.42		
$6d^77s^27p$ $1_5^o$	45 926	1.23		
$6d^77s^27p$ (51%) $1_2^o$	47 132	1.25		
$6d^77s^27p$ (65%) $2_2^o$	47 915	1.14		

(RCC) [22], multiconfigurational Dirac-Fock (MCDHF) [19], relativistic Hartree-Fock and CI [21], and relativistic pseudopotentials [20] have been used to calculate the excitation energies, ionization potentials, and oscillator strengths of Cn. Unlike the other SHEs there have also been studies on the first and second ions of Cn in [19,22]. Using the CIPT method we compared our calculations of neutral Hg and the ions Hg II and Hg III with experimental results, the results are presented in Table IV along with some results of other methods for comparison. Only a few low-energy states in the excitation spectrum of Hg I, II, and III are calculated due to the stability of the closed shells. We find agreement between the experimental and CIPT results of  $|\Delta| < 1000 \text{ cm}^{-1}$  in Table IV. The accuracy of our CIPT calculations is similar to the accuracy of previous calculations using RCC and RHF

TABLE IV. Comparison of CIPT energy-level calculations,  $E_T$ , and experimental energy levels,  $E_E$ , results for neutral Hg and ions. Where available, the experimental Landé  $g$  factors  $g_E$  are given along with calculated  $g$  factors  $g_T$ . The difference between the experimental and theoretical energies are also presented,  $\Delta_{\text{CIPT}} = E_E - E_T$ . We also present the accuracy of other methods used to calculate the spectra using relativistic coupled cluster  $\Delta_{\text{RCC}}$  and relativistic Hartree Fock,  $\Delta_{\text{RHF}}$ .

State	$E_E$ [35] ( $\text{cm}^{-1}$ )	$g_E$	$E_T$ ( $\text{cm}^{-1}$ )	$g_T$ ( $\text{cm}^{-1}$ )	$\Delta_{\text{CIPT}}$ ( $\text{cm}^{-1}$ )	$\Delta_{\text{RCC}}$ [22] ( $\text{cm}^{-1}$ )	$\Delta_{\text{RHF}}$ [21] ( $\text{cm}^{-1}$ )
Hg I							
$5d^{10}6s^2$	$^1S_0$	0	0	0			
$5d^{10}6s6p$	$^3P_0^o$	37 645	37 572	0	73	192	165
$5d^{10}6s6p$	$^3P_1^o$	39 412	39 124	1.48	288	110	74
$5d^{10}6s6p$	$^3P_2^o$	44 043	43 623	1.50	420	-156	-244
$5d^{10}6s6p$	$^3P_1^o$	54 068	52 658	1.02	1410		-194
Hg II							
$5d^{10}6s$	$^2S_{1/2}$	0.00	0.00	2.00			
$5d^96s^2$	$^2D_{5/2}$	35 515	37 278	1.20	-1763	77	
$5d^{10}6p$	$^2P_{1/2}^o$	51 486	52 130	0.67	-644	-545	
$5d^96s^2$	$^2D_{3/2}$	50 556	51 423	0.80	-867	-233	
$5d^{10}6p$	$^2P_{3/2}^o$	60 608	60 860	1.33	-252	-661	
Hg III							
$5d^{10}$	$^1S_0$	0.0	0				
$5d^96s$	$1_3$	42 850.3	43 791	1.33	-941	-865	
$5d^96s$	$1_2$	46 029.5	46 997	1.17	-968	-824	
$5d^96s$	$1_1$	58 405.8	58 538	0.50	-132	-1224	

methods as seen in Table IV. Only two states have a significantly larger discrepancy than previous calculations. In Table V the low-lying spectrum of Cn is presented and compared to other calculations. The CIPT calculations of Hg I were performed using the reference configurations  $5d^{10}6s^2$  (even states) and  $5d^96s^26p$  and  $5d^{10}6s6p$  (odd states). For Hg II we used reference states  $5d^96s^2$  and  $5d^{10}6s$  (even states) and  $5d^86s^26p$ ,  $5d^96s6p$  and  $5d^{10}6p$  (odd states). For Hg III we used reference states  $5d^86s^2$ ,  $5d^96s$ , and  $5d^{10}$  (even states) and  $5d^76s^26p$ ,  $5d^86s6p$ , and  $5d^96p$  (odd states). The same sets of reference configurations were used for the Cn I–III calculations with the appropriate principal quantum numbers (see Table VI).

TABLE V. Comparison of theoretical energy-level calculations for neutral Cn. The energy levels of this work are given by  $E_{\text{CIPT}}$  with  $g$  factors  $g_{\text{CIPT}}$ . Where available, previous atomic calculations using multiconfigurational Dirac-Fock ( $E_{\text{MCDf}}$ ) and relativistic Hartree-Fock calculations ( $E_{\text{RHF}}$ ) are presented for comparison.

State	$E_{\text{CIPT}}$ ( $\text{cm}^{-1}$ )	$g_{\text{CIPT}}$	$E_{\text{RHF}}$ [21] ( $\text{cm}^{-1}$ )	$E_{\text{MCDf}}$ [19] ( $\text{cm}^{-1}$ )
$6d^{10}7s^2$	$^1S_0$	0	0	0
$6d^97s^27p$	$1_2$	31 263	1.37	35 785
$6d^97s^27p$	$1_3$	33 857	1.10	38 625
$6d^{10}7s7p$	$^3P_0^o$	45 097	0.00	51 212
$6d^{10}7s7p$	$^3P_1^o$	47 293	1.41	52 024
$6d^97s^27p$	$^3P_2^o$	54 241	0.98	60 809

## V. ELECTRIC DIPOLE TRANSITIONS AND ISOTOPE SHIFTS

Along with the excitation spectrum we also calculated the allowed electric dipole transition rates  $A_{E1}$  between excited states and the ground state for transition frequencies  $\omega < 45\,000 \text{ cm}^{-1}$ . These are presented in Table VII. Only

TABLE VI. Comparison of theoretical energy-level calculations for Cn II and Cn III. The energy levels of this work are given by  $E_{\text{CIPT}}$  with  $g$  factors  $g_{\text{CIPT}}$ . Previous atomic calculations using relativistic coupled-cluster calculations ( $E_{\text{RCC}}$ ) are presented for comparison. The configuration weights for the strongly mixed states are also presented.

State	$E_{\text{CIPT}}$	$g_{\text{CIPT}}$	$E_{\text{RCC}}$ [22]
Cn II			
$6d^97s^2$	$^2D_{5/2}$	0	1.20
$6d^{10}7s$	$^2S_{1/2}$	11 037	2.00
$6d^97s^2$	$^2D_{3/2}$	23 760	0.80
$6d^87s^27p$	$1_{7/2}^o$	53 236	1.31
Cn III			
$6d^87s^2$	$1_4$	0	1.23
$6d^87s^2$	(52%) $1_2$	681	1.08
$6d^97s$	$1_3$	1160	1.33
$6d^{10}$	(68%) $^1S_0$	8521	0.00
$6d^97s$	$1_1$	27 029	0.50
$6d^87s7p$	$1_1^o$	64 336	1.29

TABLE VII. Strong electric dipole transition amplitudes  $D_{E1}$  and transition rates  $A_{E1}$  from the ground state to the upper odd-parity states of Ds I, Ds II, Rg I, and Rg II are presented. Isotope shift parameters  $a$ ,  $F$ , and  $\tilde{F}$  between lighter, synthesized isotopes and the theoretically metastable isotope with neutron number  $N = 184$  are also presented.

Upper state	Energy (cm <sup>-1</sup> )	$D_{E1}$ (a.u.)	$A_{E1}$ ( $\times 10^6$ s <sup>-1</sup> )	$a$ (cm <sup>-1</sup> )	$F$ ( $\frac{\text{cm}^{-1}}{\text{fm}^2}$ )	$\tilde{F}$ (cm <sup>-1</sup> )
Ds I						
$1_4^o$	21 812	0.318	0.236	64.5	5.07	37.8
$1_5^o$	24 958	0.008 46	0.000205	65.7	5.17	38.6
$1_3^o$	32 645	0.125	0.156	50.6	3.98	29.7
$2_4^o$	34 919	1.132	12.3	-183	-14.4	-108
$2_3^o$	36 404	0.0790	0.0873	64.5	5.07	37.8
$3_4^o$	39 814	0.464	3.06	85.9	6.76	50.5
$2_5^o$	40 173	2.06	50.9	-120	-9.45	-70.5
$3_5^o$	42 682	0.631	5.72	-34.1	-2.68	-20.0
$3_3^o$	42 722	0.359	2.90	-77.1	-6.07	-45.3
$4_4^o$	43 915	1.08	22.2	-27.8	-2.19	-16.3
Ds II						
$1_{7/2}^o$	37 951	0.135	0.251	49.3	3.88	28.9
$1_{9/2}^o$	39 010	0.949	10.8	-206	-16.2	-121
$2_{9/2}^o$	41 911	0.898	12.0	36.7	2.88	21.5
Rg I						
$1_{7/2}^o$	28 224	0.115	0.0753	80.9	6.15	46.0
$1_{3/2}^o$	32 677	0.487	4.20	58.1	4.42	33.0
$1_{5/2}^o$	34 398	0.374	1.92	56.9	4.33	32.3
$4P_{5/2}^o$	42 709	0.932	22.9	-235	-17.9	-134
Rg II						
$1_4^o$	42 047	0.290	1.41	69.5	5.29	39.5

these transitions are considered as they can be measured with the current experimental spectroscopy methods for heavy elements [4,38,39]. The maximum transition frequency currently accessible is  $\omega \approx 40\,000^{-1}$ [40] so states up to  $\omega = 45\,000$  cm<sup>-1</sup> are presented to account for the uncertainty in the calculations and future experimental advancements. These spectroscopic properties are some of the first to be measured and therefore theoretical predictions will aid targeted searches in future experiments.

The  $E1$  transition rates are calculated using the formula

$$A_{E1} = \frac{4}{3}(\alpha\omega)^3 \frac{D_{E1}^2}{2J+1}, \quad (4)$$

where  $J$  is the angular momentum of the upper state and  $D_{E1}$  is the  $E1$  transition amplitude. The  $E1$  transition amplitudes are calculated using a self-consistent random-phase approximation (RPA) (see Refs. [11,41] for more details). The accuracy of these calculations was discussed in Refs. [12,13] by calculating the transition rates of light analogs and comparing to experiment. It was found that while the accuracy of the  $E1$  rates was not on the same level as the energy spectrum calculations, they were in agreement to an order of magnitude. This is due to the  $\omega^3$  proportionality in Eq. (4) which drastically decreases the accuracy of  $A_{E1}$  for reasonably small deviations in accuracy of  $\omega$  (energy levels). However, as these rates are primarily used to identify promising states for experimental measurements, this level of accuracy is sufficient. All possible

strong optical  $E1$  transitions for the neutral atoms and ions considered in Secs. III and IV are presented in Table VII.

From Table VII we see there are several optically accessible states for Ds I compared to Pt I. However, few of these states have large transition rates. The transitions with the largest rates are  ${}^3F_4 \rightarrow 2_5^o$ ,  ${}^3F_4 \rightarrow 4_4^o$ , and  ${}^3F_4 \rightarrow 2_4^o$ . For Ds II the promising transitions are  ${}^4F_{9/2} \rightarrow 1_{9/2}^o$  and  ${}^4F_{9/2} \rightarrow 2_{9/2}^o$ .

Along with these strong  $E1$  transitions we also calculate the isotope shift (IS) of these energy levels. The IS is an important property as it is an indirect indicator of the effect of the nucleus on the atomic properties of the atoms. The IS can be used to find the difference in nuclear radius between two isotopes and, if the spectra of lighter neutron deficient isotopes is known, predict the spectra of heavier, metastable neutron rich isotopes. This can be used to identify long sought after metastable superheavy nuclei in the spectra of astronomical data [18,42–44]. The effect of the IS is separated into two different mechanisms: the volume shifts which dominate in SHEs [45] and the mass shift which is negligible in heavy elements. Therefore, in this work we only consider the effect of the volume shift. Using the CIPT method, we calculate the excitation spectrum of each isotope by varying the nuclear radius in the nuclear potential in the HF procedure described in Sec. II. We present three different IS parameters based on different models of the IS. The first form of the IS is

$$\delta\nu = E_2 - E_1 = a(A_2^{2\gamma/3} - A_1^{2\gamma/3}), \quad (5)$$

TABLE VIII. Successive ionization potential calculations using the CIPT method for SHEs Ds, Rg, and Cn. Calculations for the lighter analogs are also presented for comparison with experimental results. Energies marked with an asterisk (\*) denote the theoretical calculations listed in the NIST database [35]. Those values are quoted as having an uncertainty of 10 000–15 000 (cm<sup>-1</sup>).

Ion	Ground state		IP (cm <sup>-1</sup> )			Ion	Ground state		IP (cm <sup>-1</sup> )			
	Config.	Term	Expt.	CIPT	Δ		Config.	<i>J</i>	CIPT	Other		
Pt	I	5 <i>d</i> <sup>9</sup> 6 <i>s</i>	<sup>3</sup> D <sub>3</sub>	72 257.8	73 225	-967	Ds	I	6 <i>d</i> <sup>8</sup> 7 <i>s</i> <sup>2</sup>	<sup>3</sup> F <sub>4</sub>	81 933	89 984 <sup>a</sup>
	II	5 <i>d</i> <sup>9</sup>	<sup>2</sup> D <sub>5/2</sub>	149 723	150 026	-303		II	6 <i>d</i> <sup>7</sup> 7 <i>s</i> <sup>2</sup>	<sup>4</sup> F <sub>9/2</sub>	141 108	
	III	5 <i>d</i> <sup>8</sup>	<sup>3</sup> F <sub>4</sub>	234 000*	245 806	-11 806		III	6 <i>d</i> <sup>6</sup> 7 <i>s</i> <sup>2</sup>	1 <sub>2</sub>	240 185	
	IV	5 <i>d</i> <sup>7</sup>	<sup>4</sup> F <sub>9/2</sub>	347 000*	353 657	-6657		IV	6 <i>d</i> <sup>6</sup> 7 <i>s</i>	<sup>6</sup> D <sub>9/2</sub>	328 830	
Au	I	5 <i>d</i> <sup>10</sup> 6 <i>s</i>	<sup>2</sup> S <sub>1/2</sub>	74 409.11	75 776	-1367	Rg	I	6 <i>d</i> <sup>9</sup> 7 <i>s</i> <sup>2</sup>	<sup>2</sup> D <sub>5/2</sub>	90 132	98 764 <sup>a</sup> , 95 748 <sup>b</sup>
	II	5 <i>d</i> <sup>10</sup>	<sup>1</sup> S <sub>0</sub>	162 950	165 104	-2154		II	6 <i>d</i> <sup>8</sup> 7 <i>s</i> <sup>2</sup>	<sup>3</sup> F <sub>4</sub>	171 989	
	III	5 <i>d</i> <sup>9</sup>	<sup>2</sup> D <sub>5/2</sub>	242 000*	260 197	-18 197		III	6 <i>d</i> <sup>7</sup> 7 <i>s</i> <sup>2</sup>	<sup>4</sup> F <sub>9/2</sub>	250 503	
	IV	5 <i>d</i> <sup>8</sup>	<sup>3</sup> F <sub>4</sub>	363 000*	368 951	-5951		IV	6 <i>d</i> <sup>7</sup> 7 <i>s</i>	<sup>5</sup> F <sub>5</sub>	338 736	
	V	5 <i>d</i> <sup>7</sup>	<sup>4</sup> F <sub>9/2</sub>	484 000*	488 769	-4769		V	6 <i>d</i> <sup>7</sup>	<sup>4</sup> F <sub>9/2</sub>	439 861	
Hg	I	5 <i>d</i> <sup>10</sup> 6 <i>s</i> <sup>2</sup>	<sup>1</sup> S <sub>0</sub>	84 184.15	84 782	-598	Cn	I	6 <i>d</i> <sup>10</sup> 7 <i>s</i> <sup>2</sup>	<sup>1</sup> S <sub>0</sub>	97 956	105 336 <sup>a</sup> , 91 569 <sup>b</sup> , 94 609 <sup>c</sup>
	II	5 <i>d</i> <sup>10</sup> 6 <i>s</i>	<sup>2</sup> S <sub>1/2</sub>	151 284.4	152 120	-836		II	6 <i>d</i> <sup>9</sup> 7 <i>s</i> <sup>2</sup>	<sup>2</sup> D <sub>5/2</sub>	184 241	
	III	5 <i>d</i> <sup>10</sup>	<sup>1</sup> S <sub>0</sub>	277 900*	280 295	-2395		III	6 <i>d</i> <sup>9</sup> 7 <i>s</i>	<sup>3</sup> D <sub>3</sub>	260 665	
	IV	5 <i>d</i> <sup>9</sup>	<sup>2</sup> D <sub>5/2</sub>	391 600*	386 525	5075		IV	6 <i>d</i> <sup>9</sup>	<sup>2</sup> D <sub>5/2</sub>	351 903	
	V	5 <i>d</i> <sup>8</sup>	<sup>3</sup> F <sub>4</sub>	493 600*	506 264	-12 664		V	6 <i>d</i> <sup>8</sup>	<sup>3</sup> F <sub>4</sub>	451 630	
	VI	5 <i>d</i> <sup>7</sup>	<sup>4</sup> F <sub>9/2</sub>	618 000*	636 714	-18 714		VI	6 <i>d</i> <sup>7</sup>	<sup>4</sup> F <sub>9/2</sub>	566 242	

<sup>a</sup>Reference [48].

<sup>b</sup>Reference [20].

<sup>c</sup>Reference [19].

where  $A_1$  and  $A_2$  are atomic numbers for two isotopes ( $A_2 > A_1$ ),  $E_1$  and  $E_2$  are the excitation energy for  $A_1$  and  $A_2$  respectively, and  $a$  is a parameter which should be calculated for each transition. This form is based on the approximation that the isotope shift is dependent on  $R_N^{2\gamma}$  where  $\gamma = \sqrt{1 - (Z\alpha)^2}$  and the large scale trend of nuclear radius  $R_N \propto A^{1/3}$ ; see Refs. [12,46] for more details. This form of the IS is convenient for isotopes with large differences in atomic number and therefore particularly useful for predicting the spectra of metastable isotopes from lighter isotopes synthesized in laboratories. However it should be noted that the large scale trend of nuclear radius and nuclear volume is not necessarily valid for SHEs due to the nonuniform density of the nucleus. This may lead to large deviations in the calculated IS [47].

The two last forms of the IS presented are related to the root-mean-squared nuclear radius,  $R_{\text{rms}} = \sqrt{\langle r^2 \rangle}$  which is the nuclear charge radius of the nucleus and is calculated using a Fermi distribution for the nuclear density. A common form of the isotope shift is the relation between the change of atomic frequency to the change of nuclear charge radius,

$$\delta\nu = F \delta R_{\text{rms}}^2. \quad (6)$$

This formula (neglecting the mass shift) is convenient for extraction of the nuclear charge radius change from isotope shift measurements of nearby isotopes. The final form of IS we present was introduced in our previous work Ref. [12]:

$$\delta\nu = \tilde{F} \frac{R_{\text{rms},A_2}^{2\gamma} - R_{\text{rms},A_1}^{2\gamma}}{\text{fm}^{2\gamma}}, \quad (7)$$

where  $\tilde{F}$  is an IS parameter to be calculated for each transition. This form is valid for all isotope calculations and is based on the IS proportionality mentioned above,  $\delta\nu \propto \delta R_{\text{rms}}^{2\gamma}$ .

For the lighter isotope in the IS calculation, we calculated the spectra using <sup>272</sup>Ds ( $R_{\text{rms},272} = 5.8534$  fm<sup>2</sup>) and <sup>272</sup>Rg ( $R_{\text{rms},272} = 5.8534$  fm<sup>2</sup>). For the metastable isotope with  $N = 184$  we used <sup>294</sup>Ds ( $R_{\text{rms},294} = 6.039$  fm<sup>2</sup>) and <sup>295</sup>Rg ( $R_{\text{rms},295} = 6.0452$  fm<sup>2</sup>). The isotope shift associated with the strong  $E1$  transitions are presented in Table VII.

## VI. SUCCESSIVE IONIZATION POTENTIALS

In this section we calculate the successive ionization potentials for Ds, Rg, and Cn. Along with the strong dipole transitions, the IP is one of the first atomic properties to be measured in elements. The IP of elements also reveals details about its chemical and spectroscopic properties. We calculate the ionic states and ionization potentials of Ds I, II, III, IV, and Rg I, II, III, IV, V, and Cn I, II, III, IV, V, VI. To calculate the IP of each element a new basis is constructed using the  $V^{N-1}$  approximation for each successive ionization. For each of these new basis sets the CIPT method is used to calculate the energies of the ground state and an ionic state with new reference configurations. For example, to calculate the  $n$ th ionization potential of Rg ( $n = 1-5$ ) we used the reference states  $6d^{9-n}7s^2$ ,  $6d^{10-n}7s$ , and  $6d^{11-n}$  for the ionic states and for the ground states  $6d^{10-n}7s^2$ ,  $6d^{11-n}7s$ , and  $6d^{12-n}$  (for  $n = 1$  only the first two ground reference states are used). This procedure is similar for all other element IP calculations.

In Table VIII we present the successive ionization potentials of the SHEs along with analogous calculations for



lighter elements for comparison with experimental results. Comparing the CIPT IPs to the experimental values for the lighter elements we see agreement between the results with a discrepancy of a few percent where experimental results are available in Ref. [35].

The IP of some of the ionic species have been calculated previously and are included for reference in Table VIII. Comparing our results with previous calculations we see there is an agreement to within  $10\,000\text{ cm}^{-1}$ . In Ref. [19] the IPs of all the neutral atoms and ions in group 12 were calculated using an MCDF method. When compared to experimental results these values are consistently 5–10% lower than experimental values.

The results of Ref. [48] were calculated by extrapolating a term in the Hamiltonian of the relativistic Hartree-Fock potential. This extrapolation was included to agree with those of lighter analogs. However as the first ionization of lighter elements is due to the removal of a  $6s$  electron, the SHEs are ionized by first removing a  $6d$  electron. Therefore, the extrapolation in Ref. [48] may not be accurate, though the calculations agree with ours to about 10% which was a similar

agreement we found for lighter SHEs calculated in [12] using the same method.

## VII. CONCLUSION

The improved calculation and understanding of atomic properties of SHEs is important in aiding future experiments on these elements. In this paper we calculated the low-lying atomic spectrum of Ds, Rg, Cn, and their ions along with promising strong  $E1$  transitions for future experimental measurements. The isotope shift parameters calculated will hopefully facilitate the detection of nuclei from the island of stability which has been long sought after. In this paper we also calculated the successive ionization potentials of the SHEs. The ionization potential is one of the first measured properties of elements and therefore these calculations should aid in experimental studies.

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- [1] S. A. Giuliani, Z. Matheson, W. Nazarewicz, E. Olsen, P. G. Reinhard, J. Sadhukhan, B. Schuetrumpf, N. Schunck, and P. Schwerdtfeger, *Rev. Mod. Phys.* **91**, 011001 (2019).
- [2] M. Schädel, *Philos. Trans. R. Soc. London A* **373**, 20140191 (2015).
- [3] J. H. Hamilton, S. Hofmann, and Y. T. Oganessian, *Annu. Rev. Nucl. Part. Sci.* **63**, 383 (2013).
- [4] M. Laatiaoui, W. Lauth, H. Backe, M. Block, and D. Ackermann, *Nature (London)* **538**, 495 (2016).
- [5] P. Chhetri, D. Ackermann, H. Backe, M. Block, B. Cheal, C. Droese, C. E. Dullmann, J. Even, R. Ferrer, F. Giacoppo, S. Gotz, F. P. Hessberger, M. Huyse, O. Kaleja, J. Khuyagbaatar, P. Kunz, M. Laatiaoui, F. Lautenschlager, W. Lauth, N. Lemesne *et al.*, *Phys. Rev. Lett.* **120**, 263003 (2018).
- [6] T. K. Sato, M. Asai, A. Borschevsky, T. Stora, N. Sato, Y. Kaneya, and K. Tsukada, *Nature (London)* **520**, 209 (2015).
- [7] M. M. Kasliwal, D. Kasen, R. M. Lau, D. A. Perley, S. Rosswog, E. O. Ofek, K. Hotokezaka, R.-R. Chary, J. Sollerman, A. Goobar, and D. L. Kaplan, *Mon. Not. R. Astron. Soc.: Lett.* (2019).
- [8] E. Eliav, S. Fritzsche, and U. Kaldor, *Nucl. Phys. A* **944**, 518 (2015).
- [9] V. Pershina, *Nucl. Phys. A* **944**, 578 (2015).
- [10] V. A. Dzuba, J. C. Berengut, C. Harabati, and V. V. Flambaum, *Phys. Rev. A* **95**, 012503 (2017).
- [11] B. G. C. Lackenby, V. A. Dzuba, and V. V. Flambaum, *Phys. Rev. A* **98**, 022518 (2018).
- [12] B. G. C. Lackenby, V. A. Dzuba, and V. V. Flambaum, *Phys. Rev. A* **99**, 042509 (2019).
- [13] B. G. C. Lackenby, V. A. Dzuba, and V. V. Flambaum, *Phys. Rev. A* **98**, 042512 (2018).
- [14] S. Goriely, A. Bauswein, and H.-T. Janka, *Astrophys. J. Lett.* **738**, L32 (2017).
- [15] G. M. Fuller, A. Kusenkov, and V. Takhistov, *Phys. Rev. Lett.* **119**, 061101 (2017).
- [16] A. Frebel and T. C. Beers, *Phys. Today* **71**(1), 30 (2018).
- [17] B. Schuetrumpf, M. A. Klatt, K. Iida, G. E. Schröder-Turk, J. A. Maruhn, K. Mecke, and P. G. Reinhard, *Phys. Rev. C* **91**, 025801 (2015).
- [18] V. A. Dzuba, V. V. Flambaum, and J. K. Webb, *Phys. Rev. A* **95**, 062515 (2017).
- [19] J. G. Li, C. Z. Dong, Y. J. Yu, X. B. Ding, S. Fritzsche, and B. Fricke, *Eur. Phys. J. D* **44**, 51 (2007).
- [20] T. Hangele, M. Dolg, M. Hanrath, X. Cao, and P. Schwerdtfeger, *J. Chem. Phys.* **136**, 214105 (2012).
- [21] T. H. Dinh, V. A. Dzuba, and V. V. Flambaum, *Phys. Rev. A* **78**, 062502 (2008).
- [22] E. Eliav, U. Kaldor, and Y. Ishikawa, *Phys. Rev. A* **52**, 2765 (1995).
- [23] V. A. Dzuba, V. V. Flambaum, and M. G. Kozlov, *Phys. Rev. A* **99**, 032501 (2019).
- [24] H. P. Kelly, *Phys. Rev.* **136**, B896 (1964).
- [25] V. A. Dzuba, *Phys. Rev. A* **71**, 032512 (2005).
- [26] G. Breit, *Phys. Rev.* **34**, 375 (1929).
- [27] J. B. Mann and W. R. Johnson, *Phys. Rev. A* **4**, 1 (1971).
- [28] V. V. Flambaum and J. S. M. Ginges, *Phys. Rev. A* **72**, 052115 (2005).
- [29] V. A. Dzuba and V. V. Flambaum, *Hyperfine Interact.* **237**, 160 (2016).
- [30] V. M. Shabaev, I. I. Tupitsyn, and V. A. Yerokhin, *Phys. Rev. A* **88**, 012513 (2013).
- [31] S. Hofmann, V. Ninov, F. P. Heßberger, P. Armbruster, H. Folger, G. Münzenberg, H. J. Schött, A. G. Popeko, A. V. Yeremin, A. N. Andreyev, S. Saro, R. Janik, and M. Leino, *Z. Phys. A* **350**, 277 (1995).
- [32] S. Hofmann, V. Ninov, F. P. Heßberger, P. Armbruster, H. Folger, G. Münzenberg, H. J. Schött, A. G. Popeko, A. V.

- Yeremin, A. N. Andreyev, S. Saro, R. Janik, and M. Leino, *Z. Phys. A* **350**, 281 (1995).
- [33] P. J. Karol, H. Nakahara, B. W. Petley, and E. Vogt, *Pure Appl. Chem.* **73**, 959 (2001).
- [34] E. Eliav, U. Kaldor, P. Schwerdtfeger, B. A. Hess, and Y. Ishikawa, *Phys. Rev. Lett.* **73**, 3203 (1994).
- [35] A. Kramida, Yu. Ralchenko, J. Reader, and NIST ASD Team, NIST Atomic Spectra Database (ver. 5.6.1) (online), available: <https://physics.nist.gov/asd> (2019, August 14) (National Institute of Standards and Technology, Gaithersburg, MD, 2018).
- [36] S. Hofmann, I. V. Ninov, F. P. Hessberger, P. Armbruster, H. Folger, G. Münzenberg, H. J. Schött, A. G. Popeko, A. V. Yeremin, S. Saro, R. Janik, and M. Leino, *Z. Phys. A: Hadrons Nucl.* **354**, 229 (1996).
- [37] R. Eichler, N. V. Aksenov, A. V. Belozerov, G. A. Bozhikov, V. I. Chepigin, S. N. Dmitriev, and R. Dressler, *Nature (London)* **447**, 72 (2007).
- [38] M. Laatiaoui, *EPJ Web Conf.* **131**, 05002 (2016).
- [39] H. Backe, W. Lauth, M. Block, and M. Laatiaoui, *Nucl. Phys. A* **944**, 492 (2015).
- [40] M. Laatiaoui (private communication).
- [41] V. A. Dzuba, V. V. Flambaum, and S. Schiller, *Phys. Rev. A* **98**, 022501 (2018).
- [42] N. G. Polukhina, *Phys. Usp.* **55**, 614 (2012).
- [43] V. F. Gopka, A. V. Yushchenko, V. A. Yushchenko, I. V. Panov, and C. Kim, *Kinematics Phys. Celestial Bodies* **24**, 89 (2008).
- [44] V. Fivet, P. Quinet, E. Biémont, A. Jorissen, A. V. Yushchenko, and S. Van Eck, *Mon. Not. R. Astron. Soc.* **380**, 781 (2007).
- [45] D. N. Stacey, *Rep. Prog. Phys.* **29**, 171 (1966).
- [46] V. V. Flambaum, A. J. Geddes, and A. V. Viatkina, *Phys. Rev. A* **97**, 032510 (2018).
- [47] W. Nazarewicz, *Nat. Phys.* **14**, 537 (2018).
- [48] V. A. Dzuba, *Phys. Rev. A* **93**, 032519 (2016).