PHYSICAL REVIEW A **108**, 032804 (2023)

Investigating properties of heavy and superheavy atomic systems with p^3 configurations

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(Received 27 June 2023; accepted 18 August 2023; published 5 September 2023)

We have investigated the energies and spectroscopic properties such as lifetimes, Landé g_J factors, and hyperfine-structure constants of the neutral atoms P through Mc belonging to group 15, singly ionized atoms S^+ through Lv^+ of group 16, and doubly ionized atoms Cl^{2+} through Ts^{2+} of group 17 of the periodic table. These elements have np^3 configurations with $n = 3$–7, which are highly open shell and expected to exhibit strong electron-correlation effects. We have used the four-component Dirac-Coulomb Hamiltonian along with the Gaunt term and a relativistic effective core potential while employing the relativistic multireference configuration-interaction method to perform the calculations with sufficient accuracy and compare the results with the available literature data. These comparisons suggest that our predicted values, for which experimental data are not available, are reliable enough to be useful for future applications.

DOI: 10.1103/PhysRevA.108.032804

I. INTRODUCTION

There has been growing interest in studying atomic spectroscopy of ions with np^3 configurations due to their demand for use in astrophysical analysis, diagnostic tools for tokamak, laboratories, and high-temperature-fusion plasma, to name a few [1–5]. Generally, transition lines in fine-structure splitting are found in the far-ultraviolet region. However, in atomic systems with a smaller degree of ionization, such as singly and doubly ionized systems, one can observe these lines in the visible region. These lines can easily be accessed by lasers to carry out high-precision measurements in corresponding atomic systems. For example, the magnetic dipole ($M1$) transition within the fine-structure splitting of the np^3 configuration in the Bi atom was considered for measuring parity-nonconserving electric dipole amplitude [6,7]. These transitions from various atomic species are also being considered for making optical clocks [8–11].

Biémont *et al.* conducted a systematic investigation of atomic energy levels comprising np^k configurations ($k =$ 1–5), with the aim of interpreting, identifying, and analyzing many lines relevant to astrophysical and high-temperature plasmas studies [12–16]. These calculations, however, were mainly based on the approximated relativistic Hartree-Fock (RHF) method [17]. The np and np^5 configurations, containing one particle or hole in the p shells, and the np^2 and np^4 configurations, containing two particles or holes in the p shells, are comparatively easier to handle in the many-body approach than systems having np^3 configurations since there are three valence electrons present in the p shell, which can give rise to many strongly interacting configuration-interaction spaces to determine atomic wave functions. Despite the increasing availability of computing power in recent years, rigorous calculations of the properties of atomic systems with np^3 configurations still appear to be lacking. Among the limited studies, Rynkun *et al.* calculated the energy levels and radiative properties of systems with $3p^3$ configurations for S^+, Cl^{2+}, and Ar^{3+} within the P-isoelectronic sequences using the multiconfiguration Dirac-Hartree-Fock (MCDHF) method [18], Skripnikov *et al.* calculated the electronic structure of Bi using the relativistic coupled-cluster method [19], and Hussein conducted calculations for neutral phosphorus and two of its ions with $3s^23p^k$ configurations, with $k = 2$–4, using the configuration-interaction (CI) method [20].

Besides the considered p^3 systems being highly open shell with three valence electrons, they also have many occupied electrons. Thus, determining the atomic wave functions of these systems would require multiconfiguration treatment. Dealing with a multireference many-body theory with such many-electron systems would be challenging. One way to address this challenge is to utilize a hybrid method. This means that all the occupied electrons of the system can be classified into two groups, i.e., core and valence. Then, correlations

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due to the valence electrons can be treated more rigorously than the closed-core orbitals. The CI method is more suited to including correlation effects due to the valence electrons. In contrast, less computationally expensive methods like the many-body perturbation theory (MBPT) can be employed to consider correlations among the core-core electrons and core-valence electron interactions. Several groups used such a combined CI + MBPT method to study the atomic properties of a wide range of atomic systems [21–24]. Later, this hybrid approach was extended to the CI + all-order method that treats core-core and core-valence correlations using the coupled-cluster method [25].

On the other hand, all possible correlations arising from both the core and valence electrons can be treated on equal footing using the CI method. The general-active-space (GAS) technique was developed to allow participation among more electrons for producing an ample configuration space in the multireference CI (MRCI) method. It offers a comprehensive treatment for the multivalent configurations in highly open-shell systems [26–29]. Thus, this method is tailor-made for accurate studies of atomic properties of heavier open-shell systems. To carry out the calculations systematically, the active orbitals are divided into subspaces with flexible restrictions on the allowed electronic occupation and excitations in each subspace. For this reason, the performance of the MRCI method is amazing and produces fine-structure splitting of many one-valent p-, d-, and f-block atomic systems closed to the experimental values [30].

In this study, we investigate the energies and spectroscopic properties of the neutral P through Mc, singly ionized S^+ through Lv^+, and doubly ionized Cl^{2+} through Ts^{2+} atoms from groups 15–17 of the periodic table with np^3 configurations ($n = 3$–7) using the MRCI method. The complete-basis-set (CBS) limits of the energies are used to estimate uncertainties in the calculations. First, we calculate energies using the Dirac-Coulomb-Gaunt (DCG) Hamiltonian and considering the relativistic effective core potential (RECP) in the atomic Hamiltonian. We also analyze results with different combinations of basis functions to test the reliability of the calculations. Then, we report many properties, such as lifetimes, the Landé g_J factors, and the magnetic dipole (A) and electric quadrupole (B) hyperfine-structure constants, of the fine-structure partner states with np^3 configurations. We find that the forbidden transitions among these fine-structure partner states occur in the optical region. Hence, they can be used to carry out precision measurements. Some of the reported properties can also be useful in analyses of astrophysical and plasma diagnostic processes.

II. METHODS AND TECHNICAL DETAILS

We discuss the methods and procedures adopted to calculate and estimate uncertainties in the investigated properties. All the ingredients used in the computations are available with the recently released version of the DIRAC program suite [31,32]. This program is well known in the community; however, for completeness, we outline below some of its crucial points to better understand the employed approaches to determine various quantities accurately.

A. The DCG Hamiltonian

The DCG Hamiltonian in atomic units is given by

$$\hat{H} = \sum_i [c(\vec{\boldsymbol{\alpha}} \cdot \vec{\mathbf{p}})_i + (\boldsymbol{\beta} - 1)_i m_0 c^2 + V_{\text{nuc}}(r_i)] + \sum_{i<j} \left[\frac{1}{r_{ij}} - \frac{1}{2} \frac{\vec{\boldsymbol{\alpha}}_i \cdot \vec{\boldsymbol{\alpha}}_j}{r_{ij}} \right], \tag{1}$$

where $\vec{\boldsymbol{\alpha}}$ and $\boldsymbol{\beta}$ are the Dirac matrices, $\vec{\mathbf{p}}$ is the momentum operator, m_0c^2 denotes the rest mass energy of an electron with the speed of light c, and $V_{\text{nuc}}(r_i)$ is the nuclear potential. The last term in Eq. (1) represents the Gaunt interaction, which is the leading term of the Breit interaction.

First, we obtain the Dirac-Hartree-Fock (DHF) wave function for the above Hamiltonian using the correlation-consistent basis sets, dyall.aaeXz, with $X = 2$, 3, and 4 denoting the double, triple, and quadruple ξ basis sets that were developed by Dyall and coworkers [33–39]. These basis sets are optimized to account for correlations among the electrons from all core and valence shells and polarization of the d shells. They are also augmented with diffuse and tight functions designed for the p-group elements to ensure high accuracy in the calculations. For the elements with $3p$ and $4p$ valence orbitals, the nonrelativistic correlation-consistent augmented correlation-consistent polarized valence X zeta (aug-cc-pVXZ) basis sets, as developed by Dunning and coworkers [40–42], are also used in this study. These basis sets are appropriate for light elements and include a larger number of basis functions, up to 7ξ for the $3p$ elements and 5ξ for the $4p$ elements. Such a larger size of the basis function is advantageous for achieving high-precision results in the CBS limit.

B. The RECP approach

The RECP method is efficient for heavier atomic systems to determine atomic properties with reasonable accuracy, and it is known for its lower computational cost. It treats the inner-core electrons and nuclei as chemically inert entities and explicitly includes the remaining electrons (outer-core and valence electrons) in the Hamiltonian. It accounts for the dominant relativistic effects through the nonrelativistic formulation. The effective Hamiltonian in this method is given by [43–45]

$$H_v = \sum_{i=1}^{n_v} \left(-\frac{1}{2}\Delta_i + V_i^{\text{SOPP}} \right) + \sum_{i<j}^{n_v} \frac{1}{r_{ij}}, \tag{2}$$

where $n_v = Z - Q_c$ is the number of outer correlated electrons for atomic number Z and charge of the ionic core Q_c and Δ_i is the kinetic operator. In the above expression, V_i^{SOPP} is the pseudopotential (PP) seen by the outer actively correlated electrons due to the presence of the atomic core. Kim and Lee implemented a two-component spin-orbit relativistic effective core potential (SOREP) method in the DIRAC package, and it is given by [46]

$$V_i^{\text{SOPP}} = -\frac{Q_c}{r_i} + U^{\text{AREP}} + U^{\text{SO}}. \tag{3}$$

TABLE I. The general-active-space (GAS) model is adopted in the MRCI calculation. The minimum (Min) and maximum (Max) numbers of the accumulated electron occupation, the number of Kramers pairs, the corresponding function type of the Kramers pairs, and the allowed electronic excitation orders are given per GAS layer, where S, D, T, and Q represent the single, double, triple, and quadruple excitations and m represents the number of the virtual orbitals included into the GAS model.

GAS layer No.	Min	Max	Number of Kramers pairs	Function type	Allowed excitation levels
			Core10SV2SDV3SDT		
I	9	10	5	$(n-1)d$, outer core	S
II	10	12	1	ns, outer core	S, D
III	12	15	3	np, valence	S, D, T
IV	15	15	m	rest, virtual	
			Core10SDV2SDTV3SDTQ		
I	8	10	5	$(n-1)d$, outer core	S, D
II	9	12	1	ns, outer core	S, D, T
III	11	15	3	np, valence	S, D, T, Q
IV	15	15	m	rest, virtual	
			Core18SV2SDV3SDT		
I	17	18	9	$(n-1)spd$, outer core	S
II	18	20	1	ns, outer core	S, D
III	20	23	3	np, valence	S, D, T
IV	23	23	m	rest, virtual	
			V5SDTQ		
I	1	5	4	nsp, valence	S, D, T, Q
II	5	5	m	rest, virtual	

The first term represents the Coulomb interactions between the ith electron and the atomic core. The second term is the spin-average part of the PP, and the third term takes into account spin-orbit interactions. Explicitly, these potential terms are given by

$$U^{\text{AREP}} = U_L^{\text{AREP}}(r_i) + \sum_{l=0}^{L-1}\sum_{m=-l}^{l}\left[U_l^{\text{AREP}}(r_i) - U_L^{\text{AREP}}(r_i)\right]|lm\rangle\langle lm|, \tag{4}$$

such that total angular momentum j is averaged out in terms of orbital quantum numbers l and m, and the spin-orbit interaction potential is given by

$$U^{\text{SO}} = s\sum_{l=1}^{L}\frac{2}{2l+1}\Delta U_l^{\text{SOREP}}(r_i) \times \sum_{m=-l}^{l}\sum_{m'=-l}^{l}|lm\rangle\langle lm|l|lm'\rangle\langle lm'|, \tag{5}$$

with

$$U_l^{\text{AREP}}(r_i) = \sum_k C_{lk} r_i^{n_{lk}-2}\exp\left(-\alpha_{lk}r_i^2\right) \tag{6}$$

and

$$\Delta U_l^{\text{SOREP}}(r_i) = A_{lk} r_i^{n_{lk-2}}\exp\left(-\alpha_{lk}r_i^2\right)\bigg/\frac{2}{2l+1}. \tag{7}$$

In these definitions, n_{lk}, α_{lk}, C_{lk}, and A_{lk} are known as the PP parameters and are taken from the Stuttgart-Cologne PP library package.

In the present work, we consider both small-core [47–49] and large-core [43] PPs that are developed for the p-group elements. In detail, the small-core PP ECPDS10MDFSO (ECP means 'effective core potential', DS means 'Dolg Stoll', 10 means '$Q_c = 10$', M means 'multi-electron-fit', DF means 'fully relativistic', and SO means 'spin orbit') is used for As, Se$^+$, and Br^{2+}, where $Q_c = 10$ represents the $(1s-2p)$ core, while the $3s, 3p, 3d, 4s$, and $4p$ spinors are considered the outer correlated orbitals. The small-core PP ECPDS28MDFSO is used for Sb, Te$^+$, and I^{2+}, where $Q_c = 28$ represents the $(1s-3d)$ core, while the $4s, 4p, 4d, 5s$, and $5p$ spinors are taken as the outer active orbitals. The small-core PP ECPDS60MDFSO is used for Bi, Po$^+$, and At^{2+}, where $Q_c = 60$ means that $(1s-4f)$ is the core and the remaining $5s, 5p, 5d, 6s$, and $6p$ spinors are considered to be the actively correlated orbitals. In the counterpart, the large-core PPs, ECPDS28MDFSO, ECPDS46MDFSO, and ECPDS78MDFSO, are used for As to Br^{2+}, Sb to I^{2+}, and Bi to At^{2+}, respectively, where $Q_c = 28$, 46, and 78 represent $(1s-3d)$, $(1s-4d)$, and $(1s-5d)$ cores, respectively. For the superheavy elements in the $7p$ row, we choose the small-core PP ECPDS92MDFSO [50,51], where $Q_c = 92$ represents the [Rn] $5f^{14}$ core, while the $6d$, $7s$, and $7p$ shells are used to account for the correlation effects.

The RECP calculations are carried out with the help of PP-based correlation-consistent basis sets, denoted as aug-cc-pVXZ-PP, with $X =$ D, T, Q, and 5ξ, developed by Peterson *et al.* These basis functions are optimized to include the correlation of electrons from the ns, np, and $(n-1)spd$ shells and are contracted through general schemes for the p-group elements [48,52,53].

C. Different GAS models in MRCI

After the DHF calculation using the DCG Hamiltonian and RECP approximated Hamiltonian, we perform the MRCI calculation using the Kramers-restricted configuration inter-

TABLE II. Energies (cm^{-1}) of the excited states in the np^3 configuration ($n = 3$–6) obtained using the DCG Hamiltonian in the MRCI method with dyall.aaeXz basis sets adopted, with $X = 2$, 3, and 4. Differences among final and NIST values are quoted as "Diff."

	P				S^+				Cl^{2+}			
$n = 3$	$^2D_{3/2}$	$^2D_{5/2}$	$^2P_{1/2}$	$^2P_{3/2}$	$^2D_{3/2}$	$^2D_{5/2}$	$^2P_{1/2}$	$^2P_{3/2}$	$^2D_{3/2}$	$^2D_{5/2}$	$^2P_{1/2}$	$^2P_{3/2}$
$X = 2$	13478	13499	20663	20690	17307	17348	26803	26854	20838	20918	32508	32606
$X = 3$	11934	11953	19631	19659	15542	15581	25582	25632	18825	18902	30965	31064
$X = 4$	11643	11662	19305	19332	15189	15228	25179	25229	18439	18517	30535	30635
E_{CBS}	11345	11364	19143	19171	14854	14894	24992	25042	18052	18129	30277	30375
Δ_{cor}	−104	−104	−21	−18	−105	−105	−27	−25	−106	−107	−49	−47
Δ_{virt}	18	18	91	91	7	7	88	88	−5	−5	80	80
Δ_{basis}	−298	−297	−162	−161	−335	−334	−187	−187	−387	−388	−258	−260
Final	11258	11278	19212	19244	14756	14795	25053	25105	17941	18017	30307	30408
Uncertainty	316	315	187	186	351	350	208	209	402	403	275	276
NIST [58]	11361.02	11376.63	18722.71	18748.01	14852.94	14884.73	24524.83	24571.54	18052.46	18118.43	29813.92	29906.45
Diff. (%)	−0.90	−0.87	2.62	2.65	−0.65	−0.60	2.15	2.17	−0.62	−0.56	1.65	1.68
$n = 4$	As				Se^+				Br^{2+}			
	$^2D_{3/2}$	$^2D_{5/2}$	$^2P_{1/2}$	$^2P_{3/2}$	$^2D_{3/2}$	$^2D_{5/2}$	$^2P_{1/2}$	$^2P_{3/2}$	$^2D_{3/2}$	$^2D_{5/2}$	$^2P_{1/2}$	$^2P_{3/2}$
$X = 2$	12678	12997	20306	20755	15551	16167	25483	26326	17943	19006	30059	31510
$X = 3$	11325	11627	19389	19824	14079	14663	24499	25311	16298	17311	28850	30257
$X = 4$	11032	11337	19087	19530	13720	14310	24104	24930	15904	16926	28413	29840
E_{CBS}	10781	11081	18945	19382	13458	14038	23973	24785	15609	16616	28240	29649
Δ_{cor}	−87	−84	44	62	−108	−106	20	39	−138	−134	−36	−12
Δ_{virt}	−14	−12	46	53	−40	−35	0	10	−66	−58	−39	−23
Δ_{basis}	−251	−256	−142	−148	−261	−272	−131	−145	−295	−309	−173	−191
Final	10680	10985	19036	19496	13310	13896	23993	24835	15405	16425	28164	29614
Uncertainty	266	270	156	169	286	294	132	150	332	342	181	193
NIST [58]	10592.5	10914.6	18186.1	18647.5	13168.2	13784.4	23038.3	23894.8	15042	16301	26915	28579
Diff. (%)	0.82	0.65	4.67	4.55	1.07	0.81	4.14	3.93	2.41	0.76	4.64	3.62

TABLE II. (*Continued.*)

	P				S$^+$				Cl^{2+}			
$n = 3$	$^2D_{3/2}$	$^2D_{5/2}$	$^2P_{1/2}$	$^2P_{3/2}$	$^2D_{3/2}$	$^2D_{5/2}$	$^2P_{1/2}$	$^2P_{3/2}$	$^2D_{3/2}$	$^2D_{5/2}$	$^2P_{1/2}$	$^2P_{3/2}$
$n = 5$	Sb				Te$^+$				I^{2+}			
	$^2D_{3/2}$	$^2D_{5/2}$	$^2P_{1/2}$	$^2P_{3/2}$	$^2D_{3/2}$	$^2D_{5/2}$	$^2P_{1/2}$	$^2P_{3/2}$	$^2D_{3/2}$	$^2D_{5/2}$	$^2P_{1/2}$	$^2P_{3/2}$
$X = 2$	10755	12076	18857	20829	12718	14935	23374	26722	14376	17661	27489	32637
$X = 3$	9368	10617	17873	19804	11228	13302	22269	25516	12739	15817	26148	31180
$X = 4$	9011	10280	17446	19423	10769	12883	21689	25038	12266	15377	25506	30664
E_{CBS}	8770	10015	17323	19276	10530	12598	21581	24875	11994	15045	25356	30450
Δ_{cor}	−178	−206	19	49	−206	−239	−25	1	−233	−268	−90	−58
Δ_{virt}	28	32	66	84	26	34	62	82	24	33	59	82
Δ_{basis}	−241	−265	−122	−146	−238	−285	−108	−163	−272	−332	−150	−214
Final	8620	9841	17408	19410	10351	12392	21618	24958	11786	14809	25325	30474
Uncertainty	301	337	140	176	316	374	127	182	359	428	185	236
NIST [58]	8512.125	9854.018	16395.359	18464.202	10222.385	12421.854	20546.591	24032.095	11710.6	14901	24298.8	29636.6
Diff. (%)	1.26	−0.13	6.18	5.12	1.26	−0.24	5.21	3.85	0.64	−0.61	4.22	2.82
$n = 6$	Bi				Po$^+$				At^{2+}			
	$^2D_{3/2}$	$^2D_{5/2}$	$^2P_{1/2}$	$^2P_{3/2}$	$^2D_{3/2}$	$^2D_{5/2}$	$^2P_{1/2}$	$^2P_{3/2}$	$^2D_{3/2}$	$^2D_{5/2}$	$^2P_{1/2}$	$^2P_{3/2}$
$X = 2$	11857	16446	22966	34059	16970	22932	31093	47895	22971	30069	39562	62911
$X = 3$	11401	15611	22444	33564	16672	22107	30597	47404	22750	29164	38891	62227
$X = 4$	11416	15536	22299	33626	16724	21993	30353	47353	22879	29080	38648	62212
E_{CBS}	11299	15352	22211	33487	16636	21822	30301	47246	22786	28878	38549	62045
Δ_{cor}	−107	−191	−113	−110	−85	−184	−188	−159	−57	−163	−209	−149
Δ_{virt}	133	172	153	323	124	184	124	284	121	170	118	284
Δ_{basis}	−117	−184	−88	−139	−87	−171	−52	−106	−94	−201	−99	−167
Final	11324	15333	22251	33701	16675	21822	30237	47371	22850	28885	38457	62180
Uncertainty	207	316	210	368	173	311	231	342	163	310	260	361
NIST [58]	11419.039	15437.501	21660.914	33164.805								
Diff. (%)	−0.84	−0.68	2.72	1.62								

TABLE III. Energies (cm^{-1}) of the excited states in the np^3 configuration ($n = 3$–4) obtained using the DCG Hamiltonian in the MRCI method with aug-cc-pVXZ basis sets adopted, with $X = 3$, 4, and 5. Differences among the final and NIST values are shown as "Diff."

	P				S^+				Cl^{2+}			
$n = 3$	$^2D_{3/2}$	$^2D_{5/2}$	$^2P_{1/2}$	$^2P_{3/2}$	$^2D_{3/2}$	$^2D_{5/2}$	$^2P_{1/2}$	$^2P_{3/2}$	$^2D_{3/2}$	$^2D_{5/2}$	$^2P_{1/2}$	$^2P_{3/2}$
$X = 5$	11584	11603	19244	19272	15115	15154	25103	25155	18359	18436	30459	30560
$X = 6$	11549	11568	19238	19265	15066	15105	25078	25130	18274	18352	30390	30492
$X = 7$	11544	11563	19184	19212	15072	15111	25035	25086	18320	18399	30390	30490
E_{CBS}	11524	11543	19178	19205	15044	15083	25019	25069	18273	18353	30350	30451
Δ_{cor}	−51	−51	−128	−128	−49	−48	−111	−110	−67	−67	−137	−138
Δ_{basis}	−20	−20	−6	−7	−28	−28	−16	−17	−47	−46	−40	−39
Final	11473	11492	19050	19077	14995	15035	24908	24959	18206	18286	30213	30313
Uncertainty	55	55	128	128	57	55	112	111	82	81	143	143
NIST [58]	11361.02	11376.63	18722.71	18748.01	14852.94	14884.73	24524.83	24571.54	18052.46	18118.43	29813.92	29906.45
Diff. (%)	0.99	1.01	1.75	1.75	0.96	1.01	1.56	1.58	0.85	0.92	1.34	1.36
$n = 4$	As				Se^+				Br^{2+}			
	$^2D_{3/2}$	$^2D_{5/2}$	$^2P_{1/2}$	$^2P_{3/2}$	$^2D_{3/2}$	$^2D_{5/2}$	$^2P_{1/2}$	$^2P_{3/2}$	$^2D_{3/2}$	$^2D_{5/2}$	$^2P_{1/2}$	$^2P_{3/2}$
$X = 3$	11361	11580	19164	19471	14226	14648	24278	24855	16533	17276	28586	29603
$X = 4$	11038	11252	18820	19132	13786	14214	23800	24391	16071	16816	28106	29133
$X = 5$	10919	11172	18778	19140	13604	14089	23695	24365	15809	16649	27929	29085
E_{CBS}	10800	11046	18640	18998	13443	13923	23508	24175	15646	16478	27750	28894
Δ_{cor}	−38	−35	−63	−53	−31	−27	−41	−31	−37	−32	−54	−41
Δ_{basis}	−119	−126	−138	−142	−161	−166	−187	−190	−162	−171	−179	−191
Final	10762	11011	18577	18945	13412	13896	23467	24145	15610	16446	27697	28852
Uncertainty	125	131	152	152	164	168	191	192	167	174	187	196
NIST [58]	10592.5	10914.6	18186.1	18647.5	13168.2	13784.4	23038.3	23894.8	15042	16301	26915	28579
Diff. (%)	1.60	0.89	2.15	1.59	1.85	0.81	1.86	1.05	3.77	0.89	2.90	0.96

TABLE IV. Energies (cm^{-1}) of the excited states in the np^3 configuration ($n = 4$–6) obtained by using the small-core RECP potential in the MRCI method with aug-cc-pVXZ-PP basis sets adopted, with $X = 3$, 4, and 5. Differences in the final and NIST values are given as "Diff."

	As				Se$^+$				Br^{2+}			
$n = 4$	$^2D_{3/2}$	$^2D_{5/2}$	$^2P_{1/2}$	$^2P_{3/2}$	$^2D_{3/2}$	$^2D_{5/2}$	$^2P_{1/2}$	$^2P_{3/2}$	$^2D_{3/2}$	$^2D_{5/2}$	$^2P_{1/2}$	$^2P_{3/2}$
$X = 3$	11315	11576	19157	19529	14120	14641	24258	24978	16373	17298	28600	29878
$X = 4$	10986	11258	18866	19255	13691	14226	23854	24594	15890	16833	28139	29444
$X = 5$	10896	11177	18822	19225	13549	14098	23744	24506	15708	16661	27943	29274
E_{CBS}	10770	11055	18706	19116	13386	13939	23589	24355	15528	16487	27775	29113
Δ_{cor}	−34	−31	−72	−68	−33	−30	−54	−48	−33	−27	−40	−30
Δ_{basis}	−126	−122	−116	−109	−163	−159	−155	−151	−180	−174	−168	−161
Final	10736	11024	18634	19048	13353	13909	23535	24307	15495	16460	27735	29083
Uncertainty	131	125	137	128	166	162	164	159	183	176	173	164
NIST [58]	10592.5	10914.6	18186.1	18647.5	13168.2	13784.4	23038.3	23894.8	15042	16301	26915	28579
Diff. (%)	1.35	1.00	2.46	2.15	1.40	0.90	2.16	1.73	3.01	0.97	3.04	1.76
$n = 5$	Sb				Te$^+$				I^{2+}			
	$^2D_{3/2}$	$^2D_{5/2}$	$^2P_{1/2}$	$^2P_{3/2}$	$^2D_{3/2}$	$^2D_{5/2}$	$^2P_{1/2}$	$^2P_{3/2}$	$^2D_{3/2}$	$^2D_{5/2}$	$^2P_{1/2}$	$^2P_{3/2}$
$X = 3$	9419	10473	17382	18979	11296	13149	21686	24510	13076	15901	26117	30499
$X = 4$	9047	10190	17179	18913	10860	12830	21449	24476	12362	15326	25250	30021
$X = 5$	8931	10149	17170	19036	10708	12736	21361	24517	12201	15236	25145	30094
E_{CBS}	8790	10037	17086	18993	10544	12613	21271	24498	11924	15008	24796	29888
Δ_{cor}	−39	−31	−87	−73	−39	−28	−72	−54	−32	−21	−51	−33
Δ_{basis}	−141	−112	−84	−42	−164	−123	−89	−19	−277	−228	−349	−206
Final	8751	10006	16999	18920	10505	12585	21199	24444	11892	14987	24745	29855
Uncertainty	146	116	121	84	169	126	115	57	279	229	352	209
NIST [58]	8512.125	9854.018	16395.359	18464.202	10222.385	12421.854	20546.591	24032.095	11710.6	14901	24298.8	29636.6
Diff. (%)	2.81	1.54	3.68	2.47	2.76	1.32	3.18	1.71	1.55	0.57	1.84	0.74
$n = 6$	Bi				Po$^+$				At^{2+}			
	$^2D_{3/2}$	$^2D_{5/2}$	$^2P_{1/2}$	$^2P_{3/2}$	$^2D_{3/2}$	$^2D_{5/2}$	$^2P_{1/2}$	$^2P_{3/2}$	$^2D_{3/2}$	$^2D_{5/2}$	$^2P_{1/2}$	$^2P_{3/2}$
$X = 3$	9884	13709	20322	29034	14254	19468	27584	41388	20072	27288	35969	55652
$X = 4$	10824	14834	21562	31938	15589	20794	29138	44641	21256	27475	37043	58713
$X = 5$	11055	15088	21810	32585	16087	21280	29583	45755	22002	28152	37698	60250
E_{CBS}	11419	15526	22296	33718	16584	21774	30178	46976	22404	28148	38066	61339
Δ_{cor}	−3	5	−60	−6	11	10	−50	−12	34	31	−33	29
Δ_{basis}	364	438	487	1133	497	494	595	1221	402	−5	367	1089
Final	11416	15531	22236	33712	16595	21784	30128	46964	22438	28179	38033	61368
Uncertainty	364	438	491	1133	497	494	597	1221	403	31	369	1089
NIST [58]	11419.039	15437.501	21660.914	33164.805								
Diff. (%)	−0.02	0.60	2.66	1.65								

TABLE V. Energies (cm^{-1}) of the excited states in the np^3 configuration ($n = 4 - 6$) obtained using the large-core RECP potential in the MRCI method with aug-cc-pVXZ-PP basis sets adopted, with $X = 3$, 4, and 5. Differences between E_{CBS} and NIST results are given as "Diff."

	As				Se$^+$				Br^{2+}			
$n = 4$	$^2D_{3/2}$	$^2D_{5/2}$	$^2P_{1/2}$	$^2P_{3/2}$	$^2D_{3/2}$	$^2D_{5/2}$	$^2P_{1/2}$	$^2P_{3/2}$	$^2D_{3/2}$	$^2D_{5/2}$	$^2P_{1/2}$	$^2P_{3/2}$
$X = 3$	10984	11183	18637	18923	14032	14537	23996	24674	16771	16981	28255	28547
$X = 4$	10616	10818	18113	18410	13757	14245	23708	24371	16489	16793	28121	28549
$X = 5$	10795	10967	18348	18599	13777	14235	23732	24355	16179	16419	27611	27946
E_{CBS}	10620	10796	18100	18361	13704	14167	23655	24285	16098	16386	27616	28020
Δ_{basis}	−175	−171	−248	−238	−73	−68	−77	−70	−81	−33	6	75
NIST [58]	10592.5	10914.6	18186.1	18647.5	13168.2	13784.4	23038.3	23894.8	15042	16301	26915	28579
Diff. (%)	0.26	−1.09	−0.47	−1.54	4.07	2.78	2.68	1.63	7.02	0.52	2.61	−1.95
$n = 5$	Sb				Te$^+$				I^{2+}			
	$^2D_{3/2}$	$^2D_{5/2}$	$^2P_{1/2}$	$^2P_{3/2}$	$^2D_{3/2}$	$^2D_{5/2}$	$^2P_{1/2}$	$^2P_{3/2}$	$^2D_{3/2}$	$^2D_{5/2}$	$^2P_{1/2}$	$^2P_{3/2}$
$X = 3$	8818	10084	16618	18521	10166	12650	20566	24655	12811	15411	25541	29522
$X = 4$	9044	10108	16821	18396	11133	12877	21521	24129	12646	15263	25289	29353
$X = 5$	8982	10032	16707	18262	11000	12746	21286	23903	12523	15325	25297	29722
E_{CBS}	9084	10052	16805	18225	11419	12857	21713	23712	12468	15256	25191	29607
Δ_{basis}	102	20	98	−37	419	110	427	−191	−54	−69	−106	−115
NIST [58]	8512.125	9854.018	16395.359	18464.202	10222.385	12421.854	20546.591	24032.095	11710.6	14901	24298.8	29636.6
Diff. (%)	6.72	2.01	2.50	−1.29	11.71	3.50	5.68	−1.33	6.47	2.38	3.67	−0.10
$n = 6$	Bi				Po$^+$				At^{2+}			
	$^2D_{3/2}$	$^2D_{5/2}$	$^2P_{1/2}$	$^2P_{3/2}$	$^2D_{3/2}$	$^2D_{5/2}$	$^2P_{1/2}$	$^2P_{3/2}$	$^2D_{3/2}$	$^2D_{5/2}$	$^2P_{1/2}$	$^2P_{3/2}$
$X = 3$	10727	14681	20862	31235	16493	21706	29411	46393	22476	29759	38145	60854
$X = 4$	10970	14974	21213	31926	15583	20827	29133	44518	21370	27648	37247	58806
$X = 5$	10956	14931	21138	31889	15796	21036	29262	44994	21654	27889	37473	59435
E_{CBS}	11059	15060	21296	32184	15390	20644	29129	44154	21160	26980	37071	58505
Δ_{basis}	103	129	157	294	−406	−392	−133	−840	−495	−909	−402	−930
NIST [58]	11419.039	15437.501	21660.914	33164.805								
Diff. (%)	−3.15	−2.44	−1.69	−2.96								

TABLE VI. Excitation energies (EEs) in cm^{-1} and Landé g_J factors of the ground and low-lying excited states of Mc, Lv$^+$, and Ts^{2+} obtained using the DC and RECP Hamiltonians in the MRCI method and comparison with the CI+MBPT results [60]. The dyall.aae4z basis set ("aae4z") and the dyall.aae4z basis-set expansion using the procedure introduced in Ref. [61] ("aae4z$^+$") are adopted for the DCG Hamiltonian calculation, while the dyall.aae4z basis set is adopted for the RECP calculations. The numbers in parentheses are the uncertainties. Nonrelativistic results for Landé g_J factors are also given as g_J^{LS}.

			MRCI							CI+MBPT	
Atom	State	g_J^{LS}	aae4z	aae4z$^+$	Δ_+	$\Delta_{\rm cor}$	Final	g_J	RECP/aae4z	EEs	g_J
Mc	$7p^3\ ^2P^o_{3/2}$	1.3333	0	0	0	0		1.3923	0	0	1.4039
	$7p^28s\ ^2S_{1/2}$	2.0000	18533	18525	−8	62	18587(63)	2.0302	18800	18377	2.0427
	$7p^28p\ ^2P^o_{1/2}$	0.6667	26964	26946	−17	10	26957(10)	0.6668	27254	28382	0.6668
	$7p^28p\ ^2P^o_{3/2}$	1.3333	30534	30517	−16	79	30597(81)	1.3395	30767	31716	1.3449
	$7p^27d\ ^2D_{3/2}$	0.8000	32515	32513	−2	41	32554(41)	0.7969	32766	33092	0.7987
	$7p^27d\ ^2D_{5/2}$	1.2000	33240	33237	−3	61	33299(61)	1.2008	33492	33273	1.2007
	$7p^3\ ^2P^o_{3/2}$	1.3333	37289	36785	−504	−171	36615(532)	1.4380	36667	35484	1.4295
	$7p^3\ ^2D_{5/2}$	1.2000	41282	40795	−487	568	41364(748)	1.2013	40637		
	$7p^3\ ^2P^o_{1/2}$	0.6667	47123	46938	−185	−58	46879(194)	0.6663	46483		
Lv$^+$	$7p^3\ ^2P^o_{3/2}$	1.3333	0	0	0	0	0	1.3834	0		
	$7p^28s\ ^2S_{1/2}$	2.0000	40564	40398	−166	235	40633(288)	2.0308	40275		
	$7p^3\ ^2P^o_{3/2}$	1.3333	53505	53517	13	−221	53296(221)	1.4525	54136		
	$7p^28p\ ^2P^o_{1/2}$	0.6667	56295	56290	−5	207	56497(207)	0.6669	56169		
	$7p^3\ ^2D^o_{5/2}$	1.2000	58297	58309	12	−108	58201(108)	1.2006	58359		
	$7p^27d\ ^2D_{3/2}$	0.8000	58530	58527	−3	273	58800(273)	0.7941	58886		
	$7p^27d\ ^2D_{5/2}$	1.2000	61260	61252	−8	331	61582(331)	1.2020	60941		
	$7p^3\ ^2P^o_{1/2}$	0.6667	65821	65833	12	−147	65686(148)	0.6684	65833		
	$7p^28p\ ^2P^o_{3/2}$	1.3333	65869	65844	−25	146	65990(148)	1.3329	66334		
Ts^{2+}	$7p^3\ ^2P^o_{3/2}$	1.3333	0	0	0	0	0	1.3751	0.0000		
	$7p^28s\ ^2S_{1/2}$	2.0000	62950	62857	−93	337	63194(349)	2.0283	63537		
	$7p^3\ ^2P^o_{3/2}$	1.3333	71165	71194	29	−247	70947(249)	1.4554	70007		
	$7p^3\ ^2D^o_{5/2}$	1.2000	76412	76440	28	−161	76278(164)	1.1998	75230		
	$7p^27d\ ^2D_{3/2}$	0.8000	80457	80473	16	409	80882(410)	0.7925	80589		
	$7p^3\ ^2P^o_{1/2}$	0.6667	84436	84455	20	−45	84410(49)	0.6666	83510		
	$7p^27d\ ^2D_{5/2}$	1.2000	85897	85920	22	475	86395(476)	1.2002	85859		
	$7p^28p\ ^2P^o_{1/2}$	0.6667	86344	86359	15	150	86510(151)	0.6668	86507		
	$7p^28p\ ^2P^o_{3/2}$	1.3333	102032	102044	12	211	102255(211)	1.3346	102369		
	$7p^28p\ ^2F^o_{5/2}$	0.8571	112631	112649	18	237	112886(2380	0.8510	112563		

action (KRCI) code [27–29]. For the np^3 systems, we divide the active spinors into three regimes, "outer core," "valence," and "virtual," separate from the inner core and high-lying orbitals that are frozen due to their less significant contributions to the electron-correlation effects in the MRCI method.

Table I illustrates the GAS model used for the MRCI calculation for the considered np^3 systems. In Table I, "Core10" indicates the $(n-1)d$ outer core [or $(1s, 2s, 2p)$ outer core for $3p^3$], and "Core18" denotes the $(n-1)s, p, d$ outer core. The "V2" and "V3" regions correspond to the ns^2 and np^3 electrons, respectively. The remaining unoccupied spinors consist of the virtual subspace. Thus, by designing different types of GAS models, we can investigate how the results converge with an increasing level of excitations in the hierarchy due to electron-correlation effects. For example, differences in the results between Core10SV2SDV3SDT and Core18SV2SDV3SDT will reflect the variation in the results caused by the added inner-shell electron excitations through Core10 against Core18. Similarly, differences in the results between Core10SV2SDV3SDT and Core10SDV2SDTV3SDTQ will indicate the number of correlation effects included due to consideration of the higher-level excitations when level of excitation increases from S to SD in the layer-I type, from SD to SDT in the layer-II type, and from SDT to SDTQ in the layer-III type. The Core10SV2SDV3SDT, Core10SDV2SDTV3SDTQ, and Core18SV2SDV3SDT GAS models are adopted for DCG and RECP Hamiltonians with a small core for the MRCI calculations. In the large-core RECP calculation, the outer-lying electrons are limited to five, which is undertaken by the V5SDTQ GAS model, where "V5" represents the ns^2np^3 valence electrons.

D. Evaluation of energies and properties

We estimate the energies with the CBS limit $E_{\rm CBS}$; then the net energy E_X is given by

$$E_X = E_{\rm CBS} + AX^{-3}, \tag{8}$$

where X is the cardinal number for the basis sets and A is a fitting parameter as defined in Ref. [54].

The properties of interest in this study are the lifetimes, Landé g_J factors, and hyperfine-structure constants of the

TABLE VII. The Landé g_J factor for the np^3 $^4S_{3/2}$, $^2D_{3/2,5/2}$, and $^2P_{3/2,1/2}$ states ($n = 3$–4). The g_J^D and Δg_J^Q values are obtained by using the Core10SV2SDV3SDT model ($3p^3$) and the Core18SV2SDV3SDT model ($4p^3$) for the dyall.aae4z basis set. The final values (g_J^{Total}) are then given after adding the Δ_{cor} and Δ_{virt} corrections. We also use the Δ_{cor} and Δ_{virt} values to estimate the uncertainties (Uncert.).

Atom	Parameter	$^4S_{3/2}$	$^2D_{3/2}$	$^2D_{5/2}$	$^2P_{1/2}$	$^2P_{3/2}$
P	g_J^D	1.999767	0.800184	1.200500	0.666120	1.333132
	Δg_J^Q	0.009276	−0.001853	0.001861	−0.003097	0.003091
	Δ_{cor}	−0.000001	0.000298	−0.000313	−0.000519	0.000536
	Δ_{virt}	−0.000004	−0.000079	0.000069	−0.000083	0.000086
	g_J^{Total}	2.009038	0.798550	1.202117	0.662421	1.336845
	Uncert.	0.000004	0.000308	0.000321	0.000526	0.000543
S^+	g_J^D	1.999579	0.801475	1.199954	0.666360	1.332132
	Δg_J^Q	0.009274	−0.001841	0.001856	−0.003095	0.003082
	Δ_{cor}	−0.000001	−0.000082	0.000056	−0.000014	0.000040
	Δ_{virt}	−0.000005	−0.000050	0.000035	0.000016	−0.000008
	g_J^{Total}	2.008847	0.799502	1.201901	0.663267	1.335247
	Uncert.	0.000006	0.000096	0.000066	0.000022	0.000041
Cl^{2+}	g_J^D	1.999293	0.802877	1.199844	0.666449	1.330797
	Δg_J^Q	0.009272	−0.001828	0.001855	−0.003094	0.003070
	Δ_{cor}	−0.000002	−0.000050	0.000021	0.000264	−0.000235
	Δ_{virt}	−0.000007	−0.000031	0.000007	0.000002	0.000013
	g_J^{Total}	2.008556	0.800970	1.201727	0.663621	1.333645
	Uncert.	0.000008	0.000058	0.000022	0.000264	0.000235
As	g_J^D	1.996343	0.815597	1.201699	0.662240	1.323779
	Δg_J^Q	0.009245	−0.001698	0.001859	−0.003091	0.002963
	Δ_{cor}	−0.000012	−0.000290	−0.000122	−0.000286	0.000699
	Δ_{virt}	−0.000092	−0.000867	0.000973	−0.003714	0.003683
	g_J^{Total}	2.005484	0.812741	1.204408	0.655149	1.331123
	Uncert.	0.000093	0.000914	0.000981	0.003725	0.003749
Se^+	g_J^D	1.993716	0.827341	1.200270	0.665992	1.312132
	Δg_J^Q	0.009221	−0.003182	−0.001273	0.000849	0.000529
	Δ_{cor}	−0.000001	−0.000541	−0.000029	−0.000002	0.000569
	Δ_{virt}	−0.000112	0.000038	0.000169	−0.000439	0.000331
	g_J^{Total}	2.002826	0.823655	1.199137	0.666400	1.313561
	Uncert.	0.000112	0.000542	0.000171	0.000439	0.000658
Br^{2+}	g_J^D	1.989802	0.840605	1.199930	0.666474	1.302406
	Δg_J^Q	0.009186	−0.002934	−0.001173	0.000782	0.000474
	Δ_{cor}	0.000000	−0.000613	0.000001	0.000000	0.000610
	Δ_{virt}	−0.000175	0.000289	0.000023	−0.000033	−0.000116
	g_J^{Total}	1.998813	0.837346	1.198780	0.667223	1.303374
	Uncert.	0.000175	0.000678	0.000023	0.000033	0.000621

atomic states. Since we are studying only the fine-structure splitting partners of the ground-state configurations of the undertaken atomic systems, the decay channels of the excited states will mainly be carried out through the $M1$ and electric quadrupole ($E2$) forbidden transitions. Thus, determination of the lifetimes of the considered atomic states require transition probabilities due to the $M1$ and $E2$ channels, for which it is necessary to evaluate the corresponding transition amplitudes.

It can be noted that one can find options to calculate all the considered properties in the KRCI module of the DIRAC program suite [31,32] except for a few like the $M1$ and $E2$ transition matrix elements. In these cases, we use the wave functions from the KRCI method, but the one-body integrals of the $M1$ and $E2$ operators are taken from the DIRAC program by modifying it suitably. Similar approaches are also applied for the calculations of the Landé g_J factors and the electric quadrupole hyperfine-structure constants B.

The $M1$ matrix element is evaluated in this approach as

$$\langle M1\rangle_{JJ'} = \frac{1}{C_1}\langle\psi_{J\Omega_J}|\sum_i^N(\vec{\boldsymbol{\alpha}}_i \times \vec{\mathbf{r}}_i)_z|\psi_{J'\Omega_{J'}}\rangle, \tag{9}$$

while the $E2$ matrix element is evaluated as

$$\langle E2\rangle_{JJ'} = \frac{(-1)^{(J-\Omega_J)}}{C_2} \times \left\langle\psi_{J\Omega_J}\middle|\sum_i^N -\frac{3}{2}\left(|\vec{\mathbf{r}}_{i\alpha}||\vec{\mathbf{r}}_{i\beta}| - \frac{1}{3}\delta_{\alpha\beta}r_i^2\right)_{zz}\middle|\psi_{J'\Omega_{J'}}\right\rangle. \tag{10}$$

TABLE VIII. The Landé g_J factor for the np^3 $^4S_{3/2}$, $^2D_{3/2,5/2}$, and $^2P_{3/2,1/2}$ states ($n = 5$–6). The g_J^D and Δg_J^Q values are obtained using the Core18SV2SDV3SDT model for the dyall.aae4z basis set. The final values (g_J^{Total}) are then given after adding the Δ_{cor} and Δ_{virt} corrections. We also use the Δ_{cor} and Δ_{virt} values to estimate the uncertainties (Uncert.).

Atoms		$^4S_{3/2}$	$^2D_{3/2}$	$^2D_{5/2}$	$^2P_{1/2}$	$^2P_{3/2}$
Sb	g_J^D	1.9717606	0.8771228	1.2000095	0.6661579	1.2847547
	Δg_J^Q	0.0090268	−0.0022504	−0.0009005	0.0006006	0.0003426
	Δ_{cor}	0.0004467	−0.0038865	0.0001483	−0.0008985	0.0042532
	Δ_{virt}	−0.0002223	0.0002151	0.0000096	−0.0000616	0.0001004
	g_J^{Total}	1.9810118	0.8712010	1.1992670	0.6657984	1.2894509
	Uncert.	0.0004990	0.0038925	0.0001486	0.0009006	0.0042543
	Expt. 1988 [62]	1.967	0.889	1.205	0.688	1.277
	Expt. 2016 [63]				0.676	1.279
Te$^+$	g_J^D	1.9516918	0.9082274	1.1998492	0.6664472	1.2733024
	Δg_J^Q	0.0088466	−0.0016687	−0.0006675	0.0004451	0.0002440
	Δ_{cor}	0.0006675	−0.0036881	−0.0000009	−0.0000924	0.0031347
	Δ_{virt}	−0.0001875	0.0002244	−0.0000287	−0.0000538	0.0000438
	g_J^{Total}	1.9610183	0.9030950	1.1991521	0.6667461	1.2767249
	Uncert.	0.0006933	0.0036949	0.0000287	0.0001069	0.0031350
	Expt. 1974 [64]	1.93				1.27
I^{2+}	g_J^D	1.9225889	0.9454574	1.1997966	0.6664881	1.2649503
	Δg_J^Q	0.0085860	−0.0009960	−0.0003984	0.0002656	0.0001413
	Δ_{cor}	0.0007877	−0.0033382	−0.0000021	−0.0000048	0.0025506
	Δ_{virt}	−0.0001833	0.0001944	−0.0000181	−0.0000142	0.0000279
	g_J^{Total}	1.9317793	0.9413176	1.1993780	0.6667348	1.2676701
	Uncert.	0.0008088	0.0033438	0.0000182	0.0000150	0.0025507
Bi	g_J^D	1.6588424	1.2148776	1.2001881	0.6664614	1.2607733
	Δg_J^Q	0.0061725	0.0025754	0.0010320	−0.0006883	−0.0003591
	Δ_{cor}	0.0010476	−0.0006767	−0.0022391	−0.0009671	0.0024275
	Δ_{virt}	−0.0009516	0.0012311	−0.0001282	−0.0000434	−0.0004422
	g_J^{Total}	1.6651110	1.2180073	1.1988529	0.6647626	1.2623994
	Uncert.	0.0014153	0.0014049	0.0022428	0.0009680	0.0024674
	Exp. 1985[65]		1.225	1.2	0.667	
Po$^+$	g_J^D	1.5865917	1.2837211	1.2001091	0.6665329	1.2635258
	Δg_J^Q	0.0054871	0.0030615	0.0012258	−0.0008174	−0.0004311
	Δ_{cor}	0.0009360	−0.0000332	−0.0017831	−0.0020087	0.0027685
	Δ_{virt}	0.0002473	0.0004217	−0.0000078	0.0000247	−0.0006887
	g_J^{Total}	1.5932622	1.2871710	1.1995440	0.6637314	1.2651745
	Uncert.	0.0009681	0.0004230	0.0017831	0.0020089	0.0028529
At^{2+}	g_J^D	1.5334809	1.3322873	1.1999486	0.6664755	1.2678098
	Δg_J^Q	0.0049864	0.0032765	0.0013114	−0.0008746	−0.0004686
	Δ_{cor}	−0.0012440	−0.0008953	0.0014301	0.0014944	−0.0009308
	Δ_{virt}	0.0000288	−0.0077050	0.0094668	−0.0002049	−0.0009643
	g_J^{Total}	1.5372522	1.3269636	1.2121569	0.6668904	1.2654461
	Uncert.	0.0012443	0.0077568	0.0095742	0.0015084	0.0013402

Here, J (J') is the initial- (final-) state angular momentum with the projected value $\Omega_{J(J')}$, $\alpha, \beta \equiv x, y, z$, and C_1 and C_2 denote the $3j$ symbols $\left(\begin{smallmatrix} J & 1 & J' \\ -\Omega_J & 0 & \Omega_{J'} \end{smallmatrix}\right)$ and $\left(\begin{smallmatrix} J & 2 & J' \\ -\Omega_J & 0 & \Omega_{J'} \end{smallmatrix}\right)$, respectively. Then, the lifetime τ of an excited state within the np^3 configuration (in seconds) is obtained as

$$\tau = \frac{1}{\sum_{i,O} A_{fi}^O}, \tag{11}$$

where λ_{fi} (in angstroms) is the transition wavelength between the upper state f and the lower state i and A_{fi}^O is

$$A_{fi}^{M1} = \frac{2.69735 \times 10^{13}}{(2J_f + 1)\lambda_{fi}^3} S_{fi}^{M1}, \tag{12}$$

and

$$A_{fi}^{E2} = \frac{1.11995 \times 10^{18}}{(2J_f + 1)\lambda_{fi}^5} S_{fi}^{E2}, \tag{13}$$

where the $M1$ and $E2$ line strengths are given by $S_{fi}^{M1} = \langle M1 \rangle^2$ and $S_{fi}^{E2} = \langle E2 \rangle^2$, respectively.

To determine the Dirac value of the Landé g_J factor, an expectation value of a magnetic dipole operator is calculated by [55]

$$g_J^D = \frac{1}{\Omega_J} \langle \psi_{J\Omega_J} | \sum_i (\vec{\boldsymbol{\alpha}}_i \times \vec{\mathbf{r}}_i)_z | \psi_{J\Omega_J} \rangle. \tag{14}$$

TABLE IX. Lifetimes τ (s) for the np^3 $^2D_{3/2,5/2}$ and $^2P_{3/2,1/2}$ excited states. The $M1$ and $E2$ transition matrix elements are obtained by using the Core10SV2SDV3SDT model ($3p^3$) and the Core18SV2SDV3SDT model [$n(=4\text{–}6)p^3$] with the dyall.aae4z basis set, while wavelengths are estimated either from the experimental energies or from the calculated energies of the MRCI method (in Table II) when experimental values are unavailable like for Po$^+$ and At^{2+}. We also estimate uncertainties using the Δ_{cor} and Δ_{virt} values, and they are given within the parentheses.

System	Method	$^2D_{3/2}$	$^2D_{5/2}$	$^2P_{1/2}$	$^2P_{3/2}$
P	Core10SV2SDV3SDT	7170(165)	10800(316)	7.03(6)	5.29(3)
	SCI 1982 [66]	7452	11813	6.04	4.73
	MCDF 1999 [67]	6711	13545	7.98	6.01
	Empirical 1963 [68]	3378	5152	5.08	3.38
S$^+$	Core10SV2SDV3SDT	1070(1)	3510(45)	3.19(1)	1.88(1)
	MCDF 2019 [18]	1060	3780	3.10	1.86
	SCI 1982 [66]	1134	3840	3.02	1.86
	MCDF 1984 [69]	1027	2082	2.62	1.48
	MCDF 1999 [67]	980	4091	3.37	1.96
	CI 1993 [70]	810	3496	3.03	1.70
	MCDF 2006 [71]	1378	4419	3.62	2.22
	MCHF-BP 2005 [72]	1461	4936	3.46	2.16
	MCHF-BP 2010 [73]	1580	4550	3.39	2.14
Cl^{2+}	Core10SV2SDV3SDT	190(1)	1290(10)	1.40(1)	0.69(1)
	MCDF 2019 [18]	183	1350	1.41	0.70
	MCDF 1999 [67]	197	1504	1.46	0.71
	SCI 1982 [66]	207	1413	1.41	0.72
	MCDF 1984 [69]	175	784	1.21	0.59
	Empirical 1963 [68]	141	990	1.20	0.58
As	Core18SV2SDV3SDT	21(3)	248(4)	1.08(2)	0.47(1)
	Empirical 1964 [74]	13	177	0.85	0.55
	RHF 1986 [14]	12	153	0.79	0.35
	HXR 1986 [14]	12	143	0.77	0.34
Se$^+$	Core18SV2SDV3SDT	4.14(2)	64(2)	0.34(1)	0.14(1)
	RHF 1986 [14]	2.86	46	0.28	0.12
	HXR 1986 [14]	3	45	0.27	0.12
Br^{2+}	Core18SV2SDV3SDT	1.24(1)	16(1)	0.14(3)	0.05(1)
	RHF 1986 [14]	0.87	15	0.12	0.05
	HXR 1986 [14]	0.87	15	0.12	0.05
Sb	Core18SV2SDV3SDT	1.40(7)	13(1)	0.27(1)	0.10(1)
	Empirical 1964 [74]	0.90	10	0.21	0.09
	RHF 1995 [12]	0.90	9.1	0.20	0.09
Te$^+$	Core18SV2SDV3SDT	0.37(1)	3.13(1)	0.09(3)	0.034(1)
	RHF 1995 [12]	0.27	2.40	0.07	0.031
I^{2+}	Core18SV2SDV3SDT	0.19(6)	1.29(1)	0.043(6)	0.015(1)
	RHF 1995 [12]	0.106	0.797	0.153	0.014
Bi	MRCI	0.036(1)	0.151(1)	0.019(1)	0.0058(1)
	Empirical 1964 [74]	0.032	0.119	0.016	0.0058
	RHF 1996 [13]	0.025	0.087	0.0150	0.0062
Po$^+$	Core18SV2SDV3SDT	0.0107(1)	0.043(1)	0.0060(1)	0.0021(3)
	RHF 1996 [13]	0.001	0.037	0.0059	0.0024
At^{2+}	Core18SV2SDV3SDT	0.0040(1)	0.0164(1)	0.0026(2)	0.0009(2)
	RHF 1996 [13]	0.0038	0.0149	0.0026	0.0010

In the case of a free electron, it is also known that QED corrections contribute significantly to the Landé g_J factor. To include the dominant contributions from the QED effects, we estimate these corrections approximately as

$$\Delta g_J^Q = \frac{g_e - 2}{2\Omega_J}\langle\psi_{J\Omega_J}|\sum_i(\boldsymbol{\beta\Sigma}_z)_i|\psi_{J\Omega_J}\rangle, \tag{15}$$

where $\boldsymbol{\Sigma}$ is the 4×4 spin matrix and $g_e = 2.0023193$ is the free-electron Landé g factor. Therefore, the net value of the bound-electron Landé g_J factor is given by

$$g_J^{\text{Total}} = g_J^D + \Delta g_J^Q. \tag{16}$$

Precise evaluation of the hyperfine-structure constants will also test the potential of the method to determine atomic wave functions within the nuclear region accurately. The A value is estimated as the expectation of the $M1$ hyperfine operator

TABLE X. Magnetic dipole hyperfine-structure constants A (MHz) for the np^3 $^4S_{3/2}$, $^2D_{3/2,5/2}$, and $^2P_{3/2,1/2}$ states ($n = 3$–4). The numbers in parentheses are the uncertainties estimated as the root-mean-square of Δ_{cor} and Δ_{virt}. The nuclear magnetic moment μ_N value is taken from Ref. [75].

System	I	μ_N	Model	$^4S_{3/2}$	$^2D_{3/2}$	$^2D_{5/2}$	$^2P_{1/2}$	$^2P_{3/2}$
^{31}P	1/2	1.1316	Core10SV2SDV3SDT/aae4z	93.84	430.13	739.80	1998.06	430.69
			Δ_{cor}	1.70	0.74	2.71	8.88	2.16
			Δ_{virt}	19.45	9.86	32.14	77.86	20.08
			Final	115(20)	441(10)	775(32)	2085(78)	453(20)
^{33}S$^+$	3/2	0.6438	Core10SV2SDV3SDT/aae4z	38.21	141.77	244.80	652.97	143.59
			Δ_{cor}	0.45	0.54	0.87	2.74	0.87
			Δ_{virt}	5.23	2.82	9.03	22.00	5.56
			Final	44(5)	145(3)	255(9)	675(22)	150(6)
^{35}Cl^{2+}	3/2	0.8219	Core10SV2SDV3SDT/aae4z	76.63	280.75	483.47	1288.29	283.48
			Δ_{cor}	0.72	1.13	1.79	5.18	1.62
			Δ_{virt}	8.26	4.98	15.41	38.23	9.30
			Final	86(8)	287(5)	501(16)	1332(39)	294(9)
^{75}As	3/2	1.4395	Core18SV2SDV3SDT/aae4z	−75.69	383.16	646.22	1959.84	326.34
			Δ_{cor}	4.80	1.72	5.80	12.13	3.80
			Δ_{virt}	−32.70	21.13	8.88	59.84	−9.00
			Final	−104(33)	406(21)	661(11)	2032(61)	321(10)
			Expt. 1987 [76]		480(9)	725(26)	1909(14)	359(59)
^{77}Se$^+$	1/2	0.5355	Core18SV2SDV3SDT/aae4z	−120.37	660.58	1138.37	3430.49	583.02
			Δ_{cor}	6.79	1.72	7.19	16.17	4.80
			Δ_{virt}	−39.86	23.63	16.04	82.46	−4.20
			Final	−153(40)	686(24)	1162(18)	3529(84)	584(6)
^{79}Br^{2+}	3/2	2.1064	Core18SV2SDV3SDT/aae4z	−114.77	1208.43	2160.71	6411.48	1134.43
			Δ_{cor}	9.47	3.01	9.68	22.21	6.70
			Δ_{virt}	−58.46	34.09	26.58	131.64	−4.05
			Final	−164(59)	1245(34)	2197(28)	6565(134)	1137(8)

given by [56]

$$A = \frac{\mu_N}{I\Omega_j}\langle\psi_{J\Omega_J}|\sum_i^N\left(\frac{\vec{\boldsymbol{\alpha}}_i\times\vec{\mathbf{r}}_i}{r_i^3}\right)_z|\psi_{J\Omega_J}\rangle, \tag{17}$$

where μ_N and I are the nuclear magnetic moment and the nuclear spin quantum number, respectively. Similarly, the B constant is calculated as the expectation value of the electric-field gradient tensor operator as [57]

$$B = Q\langle\psi_{JJ}|\sum_i^N -\left(\frac{3|\vec{\mathbf{r}}_{i\alpha}||\vec{\mathbf{r}}_{i\beta}| - \delta_{\alpha\beta}r_i^2}{r_i^5}\right)_{zz}|\psi_{JJ}\rangle, \tag{18}$$

where Q is the nuclear electric quadrupole moment and ψ_{JJ} is known as the stretch state with $\Omega_J = J$.

III. RESULTS AND DISCUSSION

The p^3 configuration has five fine-structure splitting states, the ground state $^4S_{3/2}$ and the excited states $^2D_{3/2,5/2}$ and $^2P_{1/2,3/2}$. The excitation energies of the $^2D_{3/2,5/2}$ and $^2P_{1/2,3/2}$ states that are calculated using the DCG and RECP Hamiltonians with different types of basis sets are tabulated in Tables II–V for the $n(=3-6)p^3$ configurations. The superheavy ions with the $7p^3$ configuration have many states with the $^2P_{1/2,3/2}$ levels, separate from the other excited states such as $7p^28s$, $7p^28p$, and $7p^27d$, whose energies are given in Table VI. We compare these values with the experimental values quoted in the National Institute of Standards and Technology (NIST) database [58]. We compare the calculated energies using the DCG and RECP Hamiltonians for each type of basis set to understand the trends of the correlation effects and the accuracy of the results. The values are obtained using the dyall.aaeXz basis set with the MRCI method with the DCG Hamiltonian and are given in Table II. Convergence in the results is verified by performing calculations with $X = 2$, 3, and 4 basis sets in the Core10SV2SDV3SDT model approximation. Then, we extrapolate the E_{CBS} values using Eq. (8) and give Δ_{basis}, which are the differences between the values of E_{CBS} and those under $X = 4$. We also estimate the Δ_{cor} contributions using the Core10SDV2SDTV3SDTQ and Core18SV2SDV3SDT model calculations with the $X = 2$ basis set. Differences in the results from the Core10SV2SDV3SDT calculations with the virtual spinor cutoff values at 10 and 20 a.u. with the $X = 4$ basis set indicate the order of magnitude of the Δ_{virt} contributions. The net results listed in the "Final" rows in the Table II are taken as E_{CBS} along with the Δ_{cor} and Δ_{virt} contributions. Uncertainties in these quantities are also given.

It can be noted that a truncated MRCI method can have size-extensivity and size-consistent problems. One can find several discussions on these in Ref. [59], where simple formulas to estimate errors in the correlation energy of a system due to a size-consistent problem in the multireference single and double excited CI method is given by the Davidson-type correction ($+Q$). Our estimations of $+Q$ for the considered systems are found to be in the range of $1000-4000\,\text{cm}^{-1}$, which is quite significant. However, it is a well-known fact

TABLE XI. Magnetic dipole hyperfine-structure constants A (MHz) for the np^3 $^4S_{3/2}$, $^2D_{3/2,5/2}$, and $^2P_{3/2,1/2}$ states (n = 5–6). The numbers in parentheses are the uncertainties estimated as the root-mean-square of Δ_{cor} and Δ_{virt}. The μ_N value is taken from Ref. [75].

System	I	μ_N	Model	$^4S_{3/2}$	$^2D_{3/2}$	$^2D_{5/2}$	$^2P_{1/2}$	$^2P_{3/2}$
^{121}Sb	5/2	3.3592	Core18SV2SDV3SDT/aae4z	−401.41	613.86	1374.65	4688.08	597.11
			Δ_{cor}	45.76	−6.58	−6.81	−61.56	−2.89
			Δ_{virt}	−57.78	30.70	14.32	89.87	−5.09
			Final	−413(74)	638(31)	1382(16)	4716(109)	589(6)
			Expt. 1978 [77]		563(15)	1465(89)	4949(89)	673(42)
			Expt. 1988 [62]	−305.79(21)	565(7)	1468.98	4907.60	680(1)
^{125}Te$^+$	1/2	−0.8871	Core18SV2SDV3SDT/aae4z	375.59	−1098.16	−2778.98	−9108.30	−1288.89
			Δ_{cor}	−69.63	13.38	9.89	95.30	6.21
			Δ_{virt}	79.61	−38.44	−27.63	−161.73	11.18
			Final	386(106)	−1123(41)	−2797(30)	−9175(188)	−1272(13)
^{127}I^{2+}	5/2	2.8080	Core18SV2SDV3SDT/aae4z	−312.73	842.83	2440.26	7848.56	1167.56
			Δ_{cor}	43.14	−7.88	−6.80	−62.05	−1.55
			Δ_{virt}	−59.11	24.51	21.58	127.15	−8.04
			Final	−329(73)	859(26)	2455(23)	7914(141)	1158(8)
^{209}Bi	9/2	4.1100	Core18SV2SDV3SDT/aae4z	−502.25	−1118.46	2460.47	11005.00	456.13
			Δ_{cor}	23.52	3.57	15.80	−63.38	−42.43
			Δ_{virt}	47.32	34.36	54.16	83.08	17.39
			Final	−431(53)	−1081(35)	2530(56)	11025(105)	431(46)
			Expt. 2007 [78]	−447.52		2508.36	11272.198	
			Expt. 2000 [79]	−446.97				
^{210}Po$^+$	9/2	−0.3800	Core18SV2SDV3SDT/aae4z	−16.95	−407.26	884.31	3772.21	198.70
			Δ_{cor}	2.45	−4.25	5.39	−0.87	−7.65
			Δ_{virt}	5.82	1.81	14.08	40.07	0.93
			Final	−9(6)	−410(5)	904(15)	3811(40)	192(8)
^{210}At^{2+}	5	4.7400	Core18SV2SDV3SDT/aae4z	395.85	−2505.46	5381.35	22387.28	1321.98
			Δ_{cor}	10.83	12.65	−12.09	49.85	−19.30
			Δ_{virt}	5.95	238.11	−198.45	260.64	5.05
			Final	413(12)	−2255(238)	5171(199)	22698(265)	1308(20)

that the full CI method does not have such an issue. Thus, errors due to the size-extensivity problem can be minimized by including contributions from higher-level excitations beyond the doubles from the given reference states. The most important electronic correlation effects come from the valence triple excitations of the p^3 configurations, which have to be included rigorously. That is why we have performed calculations starting with the single, double, and triple excitations using the MRCI method. The estimated correction containing contributions from the quadruple excitations (labeled Δ_{cor}), as discussed below, is found to be small. Again, we use the multireference approach to carry out the calculations. Considering both these higher-level excitations and multireference method in the calculations can compensate a large part of the errors arising due to the size-extensivity issue. This can be verified by comparing our calculated energies with the available experimental values. Obviously, these errors can be reduced further by including contributions from even higher level excitations, which we defer to future work.

From Table II, it can be observed that our calculations for P to Bi show good agreement with the NIST data. There are discrepancies of about 1% in the calculated energy values for the $^2D_{3/2,5/2}$ states compared with the experimental values, while they are about 2%–6% for the $^2P_{1/2,3/2}$ states. Our analysis shows that the inclusion of correlation effects due to the inner-core orbitals or higher-level excitation configurations through the MRCI method does not improve the calculations substantially. However, these calculations are very sensitive to the choice of basis functions. The above energy values are obtained using the dyall.aae4z basis set; the Δ_{basis} corrections estimated due to increasing basis size are seen to be non-negligible. This implies that the discrepancies seen above for the calculated energies are mainly due to the finite-size basis functions used in the MRCI calculations. We also give the energies of the Po$^+$ and At^{2+} ions in Table II, which have $6p^3$ ground-state configurations. We cannot find any experimental data for these ions to compare with our calculations. Based on the comparison of our calculated data for other neutral, singly ionized, and doubly ionized atoms with the $n(=3\text{–}5)p^3$ ground-state configurations, we can infer uncertainties for these calculations are within 3%.

We present the excitation energies of some of the above systems with $3p^3$ and $4p^3$ configurations obtained using the aug-cc-pVXZ basis sets in the MRCI method in Table III. It should be noted that the quality of the aug-cc-pVXZ basis set is better than that of the dyall.aaeXz basis set. Therefore, aug-cc-pVXZ basis set are more suitable for carrying out calculations with the DCG Hamiltonian in the MRCI method. They can include contributions from a large number of virtual orbitals. The size of basis set increases to 7ξ for systems with 3p valence orbitals and 5ξ for systems with 4p valence orbitals. This may be the reason why the MRCI calculations using the DCG Hamiltonian match the NIST data better than the previously mentioned values that were obtained using the

TABLE XII. Electric quadrupole hyperfine-structure constants B (MHz) for the np^3 $^4S_{3/2}$, $^2D_{3/2,5/2}$, and $^2P_{3/2}$ levels of np^3 ($n = 3$–6). The numbers in parentheses are the uncertainties estimated as the root-mean-square of Δ_{cor} and Δ_{virt}. The value of the nuclear electric quadruple moment Q_s is taken from Ref. [75].

System	Q_s	Model	$^4S_{3/2}$	$^2D_{3/2}$	$^2D_{5/2}$	$^2P_{3/2}$
^{33}S$^+$	−0.678	Core10SV2SDV3SDT/aae4z	0.060	−43.178	14.011	43.027
		Δ_{cor}	0.012	0.192	0.103	−0.832
		Δ_{virt}	0.004	−1.726	−0.059	1.388
		Final	0.08(1)	−45(2)	14.1(2)	44(2)
^{35}Cl^{2+}	0.085	Core10SV2SDV3SDT/aae4z	−0.015	12.887	−2.012	−13.008
		Δ_{cor}	0.001	0.002	−0.013	0.069
		Δ_{virt}	−0.001	0.432	0.050	−0.397
		Final	−0.015(1)	13.3(4)	−1.98(5)	−13.3(4)
^{75}As	0.3	Core18SV2SDV3SDT/aae4z	−0.284	93.343	−7.654	−92.503
		Δ_{cor}	−0.015	−0.217	−0.094	1.537
		Δ_{virt}	0.074	5.123	2.365	−6.895
		Final	−0.22(7)	98(5)	−5.4(24)	−98(7)
^{77}Se$^+$	0.535	Core18SV2SDV3SDT/aae4z	−0.351	334.254	−17.122	−333.372
		Δ_{cor}	−0.004	−1.077	−0.207	3.008
		Δ_{virt}	0.094	10.243	2.712	−10.939
		Final	−0.26(9)	343(10)	−15(3)	−341(11)
^{79}Br^{2+}	0.318	Core18SV2SDV3SDT/aae4z	0.907	337.775	−12.158	−338.564
		Δ_{cor}	0.027	−0.690	0.096	1.812
		Δ_{virt}	0.058	7.905	1.565	−8.448
		Final	0.99(6)	345(8)	−11(2)	−345(9)
^{121}Sb	−0.36	Core18SV2SDV3SDT/aae4z	−1.63	−316.31	9.01	320.59
		Δ_{cor}	−0.19	9.08	−0.47	−10.58
		Δ_{virt}	−0.14	−9.90	−4.32	10.64
		Final	−1.96(23)	−317(13)	4(4)	321(15)
		Expt. 1978 [77]		−360(89)		414(36)
		Expt. 1988 [62]		−561(6)		438(30)
^{125}Te$^+$	0.58	Core18SV2SDV3SDT/aae4z	26.12	816.31	−18.76	−844.87
		Δ_{cor}	−0.28	−17.63	0.07	20.14
		Δ_{virt}	0.67	17.79	5.39	−18.99
		Final	26.5(7)	816(25)	−13(5)	−844(28)
^{127}I^{2+}	0.72	Core18SV2SDV3SDT/aae4z	104.35	1411.23	−28.14	−1516.29
		Δ_{cor}	−0.97	−22.26	−0.17	29.08
		Δ_{virt}	2.18	24.69	6.16	−27.20
		Final	106(2)	1414(33)	−22(6)	−1514(40)
^{209}Bi	−0.516	Core18SV2SDV3SDT/aae4z	−332.9	−787.7	18.6	1167.7
		Δ_{cor}	17.5	12.0	4.1	26.9
		Δ_{virt}	−10.9	−31.8	−5.3	32.4
		Final	−326.3	−807.5	17.4	1227.0
		Expt. 1985 [65]	−324(21)	−609(34)	57(7)	1025(42)
		Expt. 2007 [78]	−305.47		38.97	
		Expt. 2000 [79]	−304.30			
^{211}Po$^+$	−0.57	Core18SV2SDV3SDT/aae4z	−779.6	−1051.7	25.0	1876.5
		Δ_{cor}	25.7	18.9	12.9	20.9
		Δ_{virt}	−13.0	−28.1	−20.6	37.3
		Final	−767(29)	−1061(34)	17(24)	1935(43)
^{210}At^{2+}	0.68	Core18SV2SDV3SDT/aae4z	1504.4	1399.6	−37.1	−2955.7
		Δ_{cor}	40.7	38.4	44.3	4.7
		Δ_{virt}	17.1	37.1	5.9	−52.5
		Final	1562(44)	1475(53)	13(45)	−3003(53)

dyall.aaeXz basis set. Thus, it can be assumed that the aug-cc-pVXZ basis set is the better choice over the dyall.aaeXz basis set for the light p-group elements from the third and fourth rows of the periodic table.

We also investigate how reliably the RECP Hamiltonian gives the energies when used instead of the DCG Hamiltonian at a similar level of calculations. For this purpose, we consider the combined small-core PPs with the aug-cc-pVXZ-PP basis in the MRCI method, and the results are listed in Table IV. The use of the small-core PPs speeds up the MRCI computation significantly. In addition, we find that the contraction of the aug-cc-pVXZ-PP basis set can include more virtual orbitals in the calculation using the MRCI method. We first carry out these calculations under the Core18SV2SDV3SDT model approximation. These calculations with the $X = 3$, 4, and 5ξ basis set show excellent convergence of the results and are denoted E_{CBS}. We then improve the calculations by correlating electrons from more core orbitals under the Core18SDV2SDTV3SDTQ model approximation and considering the aug-cc-pV3Z-PP basis set. Corrections estimated in this approach are listed under Δ_{cor} in Table IV. We consider the total value as the sum of E_{CBS} and Δ_{cor}. Uncertainties in these calculations are estimated as the root-mean-square of the contributions from Δ_{basis} and Δ_{cor}, where Δ_{basis} are determined from the convergence of the results with the size of the basis functions. A comparison of these results with the NIST data suggests that the RECP results are reasonably good. For the ${}^2P_{1/2,3/2}$ states the calculated excited energies turn out to have around 2%–4% accuracy, slightly better than those obtained using the DCG Hamiltonian. The RECP results for the Po^+ and At^{2+} ions are comparable to those obtained using the DCG Hamiltonian.

In the large-core RECP approximation case, we conduct the V5SDTQ calculations with the aug-cc-pVXZ-PP basis sets for $X = 3$, 4, and 5ξ. In Table V, the final value is determined by E_{CBS}. Comparing these values with the NIST data, we find that the energies almost agree with the NIST data except for the first excited state, ${}^2D_{3/2}$. In some cases, discrepancies from these calculations lie within 5%–12%. This suggests that considering a large core in the RECP Hamiltonian is inappropriate for obtaining accurate results for systems with $n(=4-6)p^3$ configurations. Moreover, results for large-core PPs for Po^+ and At^{2+} show unusually underestimated results for the energies compared to the values obtained with small-core PPs in the RECP Hamiltonian and the results obtained using the DCG Hamiltonian.

The above exercises for estimating energies accurately in medium-heavy atomic systems were actually meant to understand the roles of various correlation effects for pursuing accurate calculations of energies in superheavy elements. In Table VI, we present the calculated energies of Mc, Lv^+, and Ts^{2+} and compare these values with the available literature data [60]. Due to the short-lived nature of the Mc, Lv, and Ts isotopes, measuring any spectroscopic properties of superheavy atoms and their ions is exceptionally challenging.

One particular aspect for which one should be cautious when trying to accurately calculate properties of superheavy elements is the adequate choice of a sufficiently large basis set. Currently, the dyall.aae4z basis set is available for performing large relativistic calculations using the DCG Hamiltonian. In addition, we adopt a procedure similar to that introduced in Ref. [61] which causes the number of the s and p primary functions to double. Then, we carry out calculations with the Core10SV2SDV3SDT model using the DCG Hamiltonian in the MRCI method. We predict the excitation energies of the states with $7p^3$, $7p^28s$, $7p^28p$, and $7p^27d$ configurations from these calculations. We find that the results from both the dyall.aae4z basis set and the dyall.aae4z basis-set expansion agree with each other. The correction due to the dyall.aae4z basis-set expansion is given under Δ_+. We also improve the calculations using the Core10SDV2SDTV3SDTQ model and the dyall.aae4z basis set. In this case, we truncate the virtual orbitals considering an energy cutoff at 2.0 a.u. These corrections are listed as Δ_{cor} in Table VI. Thus, the final calculated values follow as the sum of contributions from Δ_+ and Δ_{cor}. Similarly, the uncertainty of the final values is estimated as the root-mean-square of Δ_+ and Δ_{cor}. When comparing our calculations for Mc with those reported in Ref. [60], we find excellent agreement among the results from both calculations. Thus, we assume that our estimated values for the Lv^+ and Ts^{2+} ions are reliable and can be used for future applications. For completeness, we also perform calculations of energies of the considered superheavy systems using the RECP Hamiltonian in the MRCI method. We performed these calculations using the dyall.aae4z basis set, and the results show good agreement with results from the DCG Hamiltonian.

After analyzing the energies, we discuss below various spectroscopic properties of the undertaken atomic systems. We consider the same basis sets for producing the properties that gave reasonably accurate energies. Since the properties under investigation have different radial dependences, they are expected to show different trends of electron-correlation effects. Thus, we discuss these properties one after another.

A. Landé g_J factor

The Landé g_J factors for the calculated states with $n(=3-6)p^3$ configurations in the considered systems are determined using the MRCI wave functions obtained with the DCG Hamiltonian. These values are listed in Tables VII and VIII. Determining the accuracies of these quantities is more challenging than for the calculated energies. We use the largest basis set and include correlation effects due to inner-core orbitals to determine the Landé g_J factors of considered systems accurately. We employ the dyall.aae4z basis set in the Core10SV2SDV3SDT model ($3p^3$) and the Core18SV2SDV3SDT model [$n(=4-6)p^3$] with the DCG Hamiltonian to calculate the g_J^D and Δg_J^Q factors. Corrections from the high-lying virtual orbitals, i.e., Δ_{virt}, are estimated at the same level of approximation as for the energies. Further corrections are added through the higher-level excitations in the Core10SDV2SDTV3SDTQ model ($3p^3$) and the Core18SDV2SDTV3SDTQ model [$n(=4-6)p^3$] using the dyall.aae2z basis set. These corrections are listed as Δ_{cor}. In the end, the final value, g_J^{Total}, is determined as

$$g_J^{\text{Total}} = g_J^D + \Delta g_J^Q + \Delta_{\text{cor}} + \Delta_{\text{virt}}. \tag{19}$$

Also, we estimate the net uncertainty in the total value by taking the root-mean-square contributions of Δ_{cor} and Δ_{virt}. We find that uncertainties appear primarily in the fourth or fifth decimal place for the lighter systems but in the third decimal place for the heavier elements with $n = 5$–6. This level of precision is reasonable enough to compare our results with the available experimental data, as the measured values are precise only up to the second decimal place. Nonetheless, the reported Landé g_J factors will be interesting to study properties of the fine-structure splitting of the considered elements. They could also guide future experiments to improve the accuracy of the measurements.

B. Lifetimes of excited states

Table IX presents the calculated τ values for the ${}^2D_{3/2,5/2}$ and ${}^2P_{3/2,1/2}$ excited states with the $n(=3\text{–}6)p^3$ configuration, obtained using the same computational strategies followed to estimate the Landé g_J factors accurately. The uncertainties in the evaluated τ values are determined by combining the Δ_{cor} and Δ_{virt} corrections obtained from both the calculated $M1$ and $E2$ transition matrix elements. We compare our results with the available literature data and observed overall good agreement. One may notice from Table IX that there are significant discrepancies among various experimental τ values of the ${}^2D_{3/2,5/2}$ and ${}^2P_{3/2,1/2}$ states of P, S^+, and Cl^{2+} atoms reported in the literature. For example, for the case of S^+, a large discrepancy between theoretical and experimental data for very long-lived states has been debated in the literature using data from the astrophysical studies [2]. Our results are consistent with the semiempirical configuration-interaction (SCI) data reported in Ref. [66] and the multiconfiguration Dirac-Fock (MCDF) data reported in Refs. [18,67,69], while they disagree with the CI results from Ref. [70], the MCDF results from Ref. [71], and the multiconfiguration Hartree-Fock method with Breit-Pauli Hamiltonian (MCHF-BP) results from Refs. [72,73].

For the As neutral atom, Se^+ and Br^{2+} ions that have the $4p^3$ configuration, the Sb neutral atom, and Te^+ and I^{2+} ions with the $5p^3$ configuration, one can find very old studies of τ values using empirical approaches [74] and relativistic Hartree-plus-statistical-exchange (HXR) and RHF methods [12,65]. Our τ values show differences in the results by a factor of about 0.5 to 2.0 for the ${}^2D_{3/2,5/2}$ states, whereas excellent agreement can be found for the ${}^2P_{3/2,1/2}$ states. We also notice the τ values for the ${}^2P_{1/2}$ state of the I^{2+} ion, reported in Ref. [12], and the τ value for the ${}^2D_{3/2}$ state of the Po^+ ion, given in Ref. [13], show a considerable deviation from our results obtained using the MRCI method. The τ results for the Bi neutral atom and the Po^+ and At^{2+} ions show excellent agreement with the empirical results reported in Ref. [74] and the RHF results reported in Ref. [13].

Our study reveals that long-lived states exist, as can be seen from Table IX, due to the fine-structure splitting of the np^3 configurations such as for the ${}^2D_{3/2,5/2}$ states when n is less than 6 and the ${}^2P_{1/2,3/2}$ states when n is less than 4 for the investigated neutral atoms and the singly and doubly charged ions. Transitions from these states to the ground states of the respective systems are almost in the optical regime. Therefore, these transitions are beneficial for carrying out high-precision measurements using the respective atomic systems.

We also observe from Table IX that τ for the considered excited states of the investigated np^3-type atomic systems systematically decrease with increasing nuclear charge. This can be understood by analyzing Eqs. (11)–(13), which show that evaluation of τ of an excited state depends on both the λ_{fi} and S_{fi} values of the transitions from the respective excited state to all the lower states. We notice in our study that while the λ_{fi} values in the transitions of the considered atomic systems change marginally, their S_{fi} values become much larger with increasing nuclear charge. As a result, the decay rates of the considered excited states become faster, making their lifetimes shorter.

C. Hyperfine-structure constants

Tables X, XI, and XII present the hyperfine-structure constants A and B for the ${}^4S_{3/2}$, ${}^2D_{3/2,5/2}$, and ${}^2P_{1/2,3/2}$ states with the $n(=3\text{–}6)p^3$ configurations, which are obtained using the same computational procedure used for the evaluation of the Landé g_J and τ values. We compare our results with the experimental results (labeled "Expt.") where available. We find that the results under the Core10SV2SDV3SDT model ($3p^3$) and the Core18SV2SDV3SDT model [$n = (4-6)p^3$] combined with the dyall.aae4z basis set present reasonably accurate predictions of the A values. Further, we consider the corrections due to higher-order electron correlations and the increase in the correlated virtual orbitals, Δ_{cor} and Δ_{virt}, which are obtained using the same approach as that for the Landé g_J factors. After all these efforts, our final results are close to the available experimental values with deviations of around of 2%–10%. The largest discrepancy is seen for the ${}^4S_{3/2}$ ground state, for which the A values are very sensitive to the inclusion of correlation effects from the inner-shell electrons and the higher cutoff of the virtual orbitals, indicating that the accuracy of the results can be improved further with the inclusion of correlation effects from higher-level excitations and by including more virtual orbitals.

In contrast to the A values discussed above, we do not find that determination of the B values using the DCG Hamiltonian is very sensitive to the inclusion of the correlations from the higher-level excitations and high-lying virtual orbitals. Our results for the $5p^3$ ${}^2D_{3/2}$ and ${}^2P_{1/2}$ states of ^{121}Sb are closer to the experimental values reported in Ref. [77], but they deviate slightly from the values reported in Ref. [62]. Similarly, our results for the ${}^2S_{3/2}$, ${}^2D_{3/2,5/2}$, and ${}^2P_{3/2}$ states of ^{209}Bi show excellent agreement with the available experimental values reported in Refs. [65,78,79].

We also calculate the A and B values of the other singly and doubly charged ions with the np^3 configuration, for which no experimental results are available. Based on our analyses above for the neutral atoms, we anticipate that the accuracy of our calculated A and B values for these ions should be within 5%–20%. These predictions can help identify some of the unknown astrophysical lines that play important roles in plasma diagnosis processes.

IV. CONCLUSION

We determined the energies, lifetimes, Landé g_J factors, and hyperfine-structure constants of the fine-structure splitting states with the ground-state np^3 configurations for the neutral and singly and doubly charged p-group atoms with principal quantum number $n = 3\text{–}7$. For this purpose, we employed a multiconfiguration relativistic configuration-interaction method using a four-component Dirac-Coulomb-Gaunt Hamiltonian and relativistic Hamiltonian with core-polarization effects. Uncertainties in the energies were obtained by extrapolating the results using a complete set of basis functions and carrying out calculations that included higher-level excitations to account for more electron-correlation effects in the form of approximated Hamiltonians. Wherever available, we compared our results for the energies with the data listed in the NIST database and our predicted values for τ, the Landé g_J factors, and hyperfine-structure constants A and B with previously reported experimental data, which show excellent agreement. This suggests that the reported results for which experimental values are not available are reliable enough to use in various applications, including in analyses of astrophysical and plasma diagnostic processes.

ACKNOWLEDGMENTS

This work is supported by the National Key Research and Development Program of China (Grant No. 2021YFA1402104) and a project supported by the Space Application System of the China Manned Space Program. B.K.S. would like to acknowledge the use of the ParamVikram-1000 HPC of the Physical Research Laboratory (PRL), Ahmedabad.

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