

Spectra of barium, radium, and element 120: Application of the combined correlation-potential, singles-doubles, and configuration-interaction *ab initio* methods

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We apply a version of the recently developed approach combining the correlation-potential, linearized singles-doubles coupled-cluster, and configuration-interaction methods to the spectra of the heavy alkaline earths barium, radium, and element 120. Quantum electrodynamics radiative corrections are included. We have found excellent agreement between *ab initio* theory and experiment for the spectra of barium and radium, and we make accurate predictions for missing and unreliable data for all three atoms.

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I. INTRODUCTION

Preparatory work with the radium atom towards measurements of fundamental symmetries violations is in progress at Argonne National Laboratory (USA) [1] and Kernfysisch Versneller Instituut (The Netherlands) [2]. Studies of the parity and time-reversal violating atomic electric dipole moment (EDM) and atomic parity violation (APV) are particularly attractive in radium due to orders-of-magnitude enhancement of the effects, arising from both nuclear and electronic mechanisms: the presence of octupole deformation of the nucleus may lead to several-hundred times nuclear enhancement of the EDM in radium in the electronic ground state compared to mercury (see, e.g., [3,4]), for which the best limit on an atomic EDM has been placed [5]; the presence of anomalously close electronic levels of opposite parity may lead to orders-of-magnitude electronic enhancement of EDM effects in metastable states and APV effects in certain transitions [6,7].

High-precision atomic structure calculations will be required for interpretation of the APV and atomic EDM measurements [8]. Moreover, the measured low-lying excitation energies for radium are incomplete, and it is important to have high-precision predictions for these levels. There are already a number of theoretical works devoted to studies of fundamental symmetries violations in radium [7,9–14] and to the radium spectra, lifetimes, and hyperfine structure [15–21]. There are also recent measurements of a few transition frequencies and lifetimes [22–24]. In this work we use a recently developed approach that combines the correlation-potential, singles-doubles coupled-cluster, and configuration-interaction methods [25] to the radium spectra. We have found unprecedented agreement between theory and experiment for most levels using this *ab initio* method.

The heavier electronic homologue of radium is element 120. Efforts to synthesize this element are underway at the GSI heavy-ion facility (Germany), at the Joint Institute for Nuclear Research (Russia), and at RIKEN (Japan) (see, e.g., Ref. [26]). This element lies within the predicted island of stability, a region of increased stability against nuclear decay close to the next doubly magic shell closures $Z = 114$, 120, or 126 and $N = 172$ or 184, depending on the model [27]. If $Z = 120$ is the next closed proton shell, significantly increased stability is expected for this element. Enhanced stability could make atomic and chemical studies of this element possible. Already, chemical studies involving the superheavy element Sb ($Z = 106$) have proved successful [28]. The current calculations

for E120 extend the spectral range considered in previous works [29–31].

We also perform calculations for the lighter electronic homologue barium, as this can be used to gauge the accuracy for the heavier elements. The method used in this work has already been applied to the low-lying levels of barium in Ref. [25]. Here we extend the application to the excitation energies of the lowest 31 levels.

II. METHOD OF CALCULATION

We use an approach that is based on the combination of several different many-body methods: the correlation-potential (CP), linearized singles-doubles coupled-cluster (SD), and configuration interaction (CI) methods. It may be referred to as the CP+SD+CI method. This method was recently developed by Dzuba in Ref. [25] and is similar to the combined SD+CI method developed by Safronova *et al.* [32].

The CP+SD+CI and SD+CI methods are essentially based on the method combining many-body perturbation theory and the configuration interaction (MBPT+CI) [33], which has proven to be one of the most computationally efficient and accurate approaches for calculations involving heavy atoms with several valence electrons. These methods differ in their treatment of the valence-core correlations and the screened Coulomb interaction (valence-core-valence correlations), as we explain below.

Barium, radium, and element 120 have two valence electrons above a closed electronic core. We wish to find the eigenvalues and eigenvectors of the effective Hamiltonian for the two valence electrons

$$H^{\text{CI}} = h_1(r_1) + h_1(r_2) + h_2(r_1, r_2), \quad (1)$$

by diagonalizing H^{CI} with respect to wave functions constructed from linear combinations of two-electron Slater determinants; the Slater determinants are formed from relativistic Hartree-Fock orbitals found in the core of $N - 2$ electrons. Here h_1 contains all one-electron terms of the many-electron problem and h_2 contains all two-electron terms. The one-electron terms are

$$h_1 = c\alpha \cdot \mathbf{p} + (\beta - 1)mc^2 + V_{\text{nuc}} + V_{\text{HF}}^{(N-2)} + \Sigma_1, \quad (2)$$

where α and β are Dirac matrices, V_{nuc} is the nuclear potential (we use the two-parameter Fermi distribution for the nuclear density), $V_{\text{HF}}^{(N-2)}$ is the self-consistent Hartree-Fock potential

of the $N - 2$ electrons making up the electronic core, and Σ_1 is the correlation potential which accounts for the correlations between a single valence electron and the core. For E120, the choice of the nuclear parameters is important; for our Fermi distribution, we use a nuclear radius of $r = 8.0$ fm and nuclear thickness $t = 2.0$ fm, corresponding to a root-mean-square radius $r_{\text{rms}} \approx 6.42$ fm. These are the parameters we used in our previous calculation [29], and we make this choice again for easy comparison with that work.

The two-electron terms h_2 consist of the Coulomb interaction and the two-electron correlation operator Σ_2 (the screened Coulomb interaction):

$$h_2(r_1, r_2) = \frac{e^2}{|r_1 - r_2|} + \Sigma_2(r_1, r_2). \quad (3)$$

In the MBPT+CI method, both Σ_1 and Σ_2 are calculated using MBPT; they are often calculated in only second order in the Coulomb interaction. We have demonstrated before that using the all-order correlation potential Σ_1^∞ in place of the second-order correlation potential $\Sigma_1^{(2)}$ leads to significantly improved accuracy [19]. We refer to this latter approach, with the all-order Σ_1^∞ , as the CP+CI method. In the SD+CI method [32], both Σ_1 and Σ_2 are found from all-order linearized singles-doubles coupled-cluster equations.

In the current CP+SD+CI approach, we calculate the all-order Σ_1^∞ using the Feynman diagram technique, while the screening of the Coulomb interaction Σ_2 is found from the SD method. In this way, we include important classes of many-body diagrams to all orders in the Coulomb interaction, both for Σ_1 and Σ_2 . It was shown in Ref. [25] that high accuracy in excitation energies can be obtained with this choice.

In the calculation of Σ_1 , the Feynman diagram technique is used to include two classes of diagrams to all orders in the Coulomb interaction for the *direct* part: the electron-electron Coulomb screening and the hole-particle interaction inside the internal loops [34]. The *exchange* part is evaluated in second order in the Coulomb interaction by calculation of the corresponding Goldstone diagrams. Screening is taken into account in a simplified way, by multiplying the Coulomb integrals by factors found from the direct diagrams (more on this below). There is another series of diagrams, referred to as “ladder diagrams,” that are calculated using singles-doubles-type equations [35]; the corresponding corrections to the valence energies are added to the CI matrix.

Screening factors for the exchange diagrams are found by taking the ratio of the expectation value for the direct part of $\Sigma_1^{\infty, ee}$ (with the dominant all-orders electron-electron screening considered) to the expectation value for the direct part of $\Sigma_1^{(2)}$ for each multipolarity k , that is, $f_k = \langle v | \Sigma_{\text{dir}, k}^{\infty, ee} | v \rangle / \langle v | \Sigma_{\text{dir}, k}^{(2)} | v \rangle$. The corresponding factors for Ba are shown in the first row of Table I. Later, as a test of our accuracy, we consider the effect of using a different set of screening factors f_k^{hp} , found by considering both the dominant electron-electron screening and the hole-particle interaction series of diagrams; these factors are listed in the second row of Table I.

Note that we used slightly different factors for f_k in different approximations (with or without Breit or QED corrections) as well as slightly different factors for different atoms (Ba, Ra,

TABLE I. Factors for Ba used to mimic higher-order screening for exchange diagrams, $f_k = \langle v | \Sigma_{\text{dir}, k}^{\infty, ee} | v \rangle / \langle v | \Sigma_{\text{dir}, k}^{(2)} | v \rangle$ and $f_k^{\text{hp}} = \langle v | \Sigma_{\text{dir}, k}^{\infty, ee} | v \rangle / \langle v | \Sigma_{\text{dir}, k}^{(2)} | v \rangle$; k is the multipolarity of the Coulomb interaction.

$k/$	0	1	2	3	4	5	6	7	8	9
f_k	0.73	0.61	0.83	0.91	0.99	1.05	1.10	1.00	1.00	1.00
f_k^{hp}	0.86	0.73	0.97	1.02	1.07	1.11	1.15	1.00	1.00	1.00

E120). They differ by a few percent at most, and as their precise values are not of general interest we do not present them here.

We refer the reader to Ref. [25] for details regarding the calculation of Σ_2 .

In this work we quantify the corrections associated with inclusion of the Breit interaction and the quantum electrodynamics radiative corrections. The Breit interaction is considered at the relativistic Hartree-Fock (RHF) level. The radiative corrections are taken into account through the addition of a local radiative potential [36] to the nuclear potential. This radiative potential method provided a breakthrough in the ability for radiative corrections to be included into the many-body problem in heavy atoms. We refer the reader to Ref. [36] for details about this method. The radiative potential method has since been implemented in a number of works, including (with a minor modification to one of the fitting factors in the radiative potential) Refs. [37,38], where the radiative potential was added to the atomic many-body package GRASP [39,40].

The upper and lower radial components of the relativistic Hartree-Fock orbitals in the V^{N-2} potential are expanded in a basis of B splines of order $k = 9$ [41]. We use 40 B splines for Ba and Ra and 50 B splines for E120 confined to a cavity of radius 40 a.u. We perform the calculations for the exchange part of the correlation potential, the ladder diagrams, and Σ_2 using the lowest 30 states in each partial wave up to $l = 6$ for the intermediate excitations. We include the correlation potential Σ_1 for the valence levels up to $l = 4$ and Σ_2 for the valence levels up to $l = 3$. At the CI stage of the calculations, the basis for Ba and Ra (and E120) consists of the lowest 14 (18) valence states in each partial wave up to $l = 4$.

To quantify the size of the Breit and QED corrections, we have carried out three runs of the calculations, for both the ions and the neutral divalent atoms: with neither Breit nor QED, with Breit and without QED, and with both Breit and QED. As the basis is determined by the Hartree-Fock orbitals, and Breit and QED corrections enter at this level, we have used a different basis set for each of these runs. For each run, one basis is used for *all* aspects of the many-body problem: CP, SD, and CI.

III. RESULTS

Our calculations begin for the ions Ba^+ , Ra^+ , and E120^+ . The correlation potential Σ_1 that describes the valence-core correlations is the same for the monovalent ions above as for the divalent atoms Ba, Ra, and E120 when we perform the RHF calculations in the field of the $N - 2$ electrons of the core. Therefore, the quality of the spectra for the ions is a good indication of the quality of the correlation potential Σ_1 [19].

TABLE II. Ionization energies for the lowest states in each wave to $l = 3$ for Ba^+ , with units in cm^{-1} .

State	RHF	$+\Sigma_1^\infty$	Lad.	Breit	QED	Total	Expt. ^a	Δ
$6s_{1/2}$	75 340	80 808	-156	-22	-45	80 585	80 686	-101
$5d_{3/2}$	68 139	76 466	-763	34	36	75 773	75 812	-39
$5d_{5/2}$	67 665	75 622	-765	57	32	74 946	75 011	-65
$6p_{1/2}$	57 266	60 591	-128	-36	5	60 432	60 425	7
$6p_{3/2}$	55 873	58 865	-118	-16	3	58 734	58 734	0
$4f_{5/2}$	28 213	32 180	-32	117	32	32 297	32 428	-131
$4f_{7/2}$	28 222	31 989	-32	126	28	32 112	32 203	-91

^aNIST data [42].

A. Ions

Results for the ionization energies of the lowest partial waves up to $l = 3$ for the ions Ba^+ , Ra^+ , and E120^+ are presented in Tables II, III, and IV, respectively. We separate the contributions arising from inclusion of the correlation potential Σ_1^∞ (without ladder diagrams), ladder diagrams “Lad.,” the Breit interaction, and QED radiative corrections.

Absolute differences of our final results from experiment are listed in the last column under “ Δ .” These differences for Ba^+ and Ra^+ are very small, on the order of $10 - 100 \text{ cm}^{-1}$, with the largest difference $|\Delta| \approx 160 \text{ cm}^{-1}$. We expect a similar level of agreement for E120^+ .

We can see from a comparison of the final results “Total” in Tables II–IV the effect of the relativistic contraction of the s and $p_{1/2}$ orbitals in the heavier homologues, which in turn screen and push out the orbitals with higher angular momenta.

Inclusion of the ladder diagrams is very important for reaching good agreement for the d levels. The d orbitals are very low lying in the ions and play a big role in the low-lying spectra of the neutral divalent atoms. The size of the ladder diagram contribution decreases as we go from Ba^+ to E120^+ , as the d orbitals are pushed out, while the contributions for s and p levels increase.

The contributions from Breit and QED are roughly of the same magnitude, and generally increase with higher Z . The QED corrections exceed 100 cm^{-1} for the s levels for E120^+ , while they are negligible for the p waves. The largest Breit corrections we see are for the f levels, almost reaching 200 cm^{-1} . Interestingly, these f -wave corrections are mostly determined by many-body effects through the inclusion of Σ_1^∞ , and they are sensitive to the choice of the correlation potential.

TABLE III. Ionization energies for the lowest states in each wave to $l = 3$ for Ra^+ , with units in cm^{-1} .

State	RHF	$+\Sigma_1^\infty$	Lad.	Breit	QED	Total	Expt. ^a	Δ
$7s_{1/2}$	75 898	82 010	-219	-21	-87	81 684	81 842	-158
$6d_{3/2}$	62 356	70 242	-620	46	38	69 707	69 758	-51
$6d_{5/2}$	61 592	68 518	-643	67	31	67 973	68 099	-126
$7p_{1/2}$	56 878	60 739	-182	-59	2	60 499	60 491	8
$7p_{3/2}$	52 906	55 771	-140	-18	-2	55 611	55 633	-22
$5f_{5/2}$	28 660	32 768	-74	109	32	32 835	32 854	-19
$5f_{7/2}$	28 705	32 542	-76	107	27	32 600	32 570	30

^aNIST data, Ref. [42].TABLE IV. Ionization energies for the lowest states in each wave to $l = 3$ for E120^+ , with units in cm^{-1} .

State	RHF	$+\Sigma_1^\infty$	Lad.	Breit	QED	Total
$8s_{1/2}$	83 168	90 105	-520	-108	-129	89 349
$8p_{1/2}$	60 027	65 475	-379	-141	-9	64 946
$7d_{3/2}$	56 620	64 841	-593	51	58	64 357
$7d_{5/2}$	56 413	62 684	-625	46	46	62 151
$8p_{3/2}$	49 295	52 017	-179	-18	-7	51 812
$6f_{5/2}$	29 734	36 907	-211	186	97	36 978
$6f_{7/2}$	29 909	36 252	-219	169	77	36 279

It is worthwhile pointing out that the radiative potential [36] was found by fitting to the s and p levels for the hydrogenlike ions; it was not fitted to higher waves. The radiative QED corrections for the d and f waves, however, largely arise due to many-body effects, namely, core relaxation and the correlation potential. Core relaxation corresponds to alteration of the electronic core due to self-consistent solution of the RHF equations with the radiative potential included. The largest part of the core relaxation correction to the valence level shift occurs as a result of radiative corrections to s orbitals in the core, which are well fitted.

We have previously calculated the spectra of these ions for s and p levels, including estimates of Breit and radiative corrections [43]; more recently the spectra was calculated in Ref. [44] for the lowest s , p , and d levels, this time with the contribution from ladder diagrams, also.

B. Divalent atoms

In Tables V–VII we present our results for the ionization potentials (removal of one s electron, IP1, and removal of both s electrons, IP1+IP2) and excitation energies for the lowest 31 levels for Ba, lowest 40 levels for Ra, and lowest 25 levels for E120. Results presented under the column “CP^{nl}+SD+CI” mean that the all-orders correlation potential Σ_1^∞ is included (though ladder diagrams are not taken into account; the superscript “nl” is short for “no ladder”) and that the all-orders Σ_2 is included (calculated using the SD method). Contributions from ladder diagrams, Breit, and QED radiative corrections appear in the following columns.

Our final results are presented under the column “Total,” and the column “ Δ_{Expt} ” gives the deviation of these results from experiment, $\Delta_{\text{Expt}} = \text{Total} - \text{Expt}$. Results of other calculations are given in the tables, also. In particular, we have presented the most precise *ab initio* calculations available. These include different versions of coupled cluster [18,30,31,45], CP+CI [29], and SD+CI [32]. For the higher levels, where there are only limited data available, we also present for Ba and Ra the results of semiempirical CP+CI calculations [20].

1. Barium

For Ba, it is seen that the ladder diagrams give a contribution to the excitation energies of about 500 cm^{-1} for configurations containing a single $5d$ orbital, that is for $6s5d$ and $5d6p$ (excluding the very highest level). For the $5d^2$ configuration,

TABLE V. Ionization potentials (removal of one electron, IP1, and both electrons, IP1+IP2) and excitation energies for Ba. CP^{nl}+SD+CI excludes ladder diagrams, Breit, and QED; these corrections are given in subsequent columns. $\Delta_{\text{Expt}} = \text{Total} - \text{Expt}$. Results of other calculations are presented in the final column. Units are in cm^{-1} .

Conf.	Term	J	CP ^{nl} +SD+CI	Ladder	Breit	QED	Total	Expt. ^a	Δ_{Exp}	Other	
IP1	$6s^1$	2S	1/2	42 097	-173	122	-19	42 027	42 035	-8	42 444, ^b 42 120, ^c
IP1+IP2	$6s^0$	1S	0	122 905	-329	100	-64	122 612	122 721	-109	122 954, ^c 123 363, ^d 123 869 ^e
$6s5d$	3D	1	8460	575	-70	-60	8905	9034	-129	9117, ^b 8687, ^c 9249, ^d 9077 ^e	
		2	8704	576	-68	-59	9153	9216	-63	9296, ^b 8875, ^c 9441, ^d 9369 ^e	
		3	9066	576	-61	-57	9524	9597	-73	9677, ^b 9279, ^c 9840, ^d 9830 ^e	
$6s5d$	1D	2	10 996	589	-62	-66	11 457	11 395	62	11 426, ^b 11 081, ^c 11 727, ^d 11 871 ^e	
$6s6p$	$^3P^0$	0	12 351	-33	27	-35	12 310	12 266	44	12 357, ^b 12 099, ^c 12 556, ^d 12 668 ^e	
		1	12 706	-33	26	-35	12 664	12 637	27	12 728, ^b 12 474, ^c 12 919, ^d 12 947 ^e	
		2	13 603	-41	25	-32	13 555	13 515	40	13 610, ^b 13 365, ^c 13 819, ^d 13 449 ^e	
$6s6p$	$^1P^0$	1	17 887	107	11	-41	17 964	18 060	-96	18 170, ^b 17 943, ^c 18 292, ^d 20 077 ^e	
$5d^2$	3F	2	19 920	1142	-119	-110	20 833	20 934	-101	21 017 ^b	
		3	20 142	1146	-115	-108	21 065	21 250	-185	21 338 ^b	
		4	20 636	1145	-109	-106	21 566	21 624	-58	21 714 ^b	
		2	21 545	545	-46	-96	21 948	22 065	-117	22 238 ^b	
$5d6p$	$^3F^0$	3	22 436	538	-42	-93	22 839	22 947	-108	23 116 ^b	
		4	23 286	534	-39	-91	23 690	23 757	-67	23 950 ^b	
		2	22 182	996	-86	-103	22 989	23 062	-73	23 077 ^b	
$5d6p$	$^1D^0$	2	22 607	543	-48	-94	23 008	23 074	-66	23 289 ^b	
$5d^2$	3P	0	21 985	1001	-88	-104	22 794	23 209	-415	23 213 ^b	
		1	22 118	1022	-90	-104	22 946	23 480	-534	23 500 ^b	
		2	22 897	1003	-81	-100	23 719	23 919	-200	23 950 ^b	
		1	23 635	541	-61	-98	24 017	24 192	-175	24 474 ^b	
		2	23 992	545	-58	-97	24 382	24 532	-150	24 817 ^b	
$5d^2$	1G	3	24 460	543	-56	-95	24 852	24 980	-128	25 264 ^b	
		4	24 328	1069	-89	-103	25 205			24 300(300), ^f 24 684 ^b	
		0	25 115	507	-54	-94	25 474	25 642	-168	25 886 ^b	
$5d6p$	$^3P^0$	1	25 183	503	-51	-92	25 543	25 704	-161	25 947 ^b	
		2	25 466	512	-46	-90	25 842	25 957	-115	26 203 ^b	
		1	26 253	-135	28	-15	26 131	26 160	-29	26 573 ^b	
$6s7s$	3S	1	26 253	-135	28	-15	26 131	26 160	-29	26 573 ^b	
$5d^2$	1S	0	25 144	612	-28	-70	25 658	26 757	-1099	26 034 ^g	
$5d6p$	$^1F^0$	3	26 343	498	-56	-94	26 691	26 816	-125	26 968 ^b	
$6s7s$	1S	0	28 192	55	10	-37	28 220	28 230	-10	28 583 ^b	
$5d6p$	$^1P^0$	1	28 351	210	-15	-59	28 487	28 554	-67	28 788 ^b	

^aNIST data [42].

^bIHFSCC [18].

^cCP+CI [29]. IP1 found in combination with the calculation for the ion [43].

^dSD+CI [32].

^eFSCC [45].

^fEstimated in the experimental work of Palenius [46].

^gSemiempirical CP+CI [20].

the contribution amounts to roughly double this, $\approx 1000 \text{ cm}^{-1}$. The ladder diagrams give a small correction to the other levels.

The Breit and radiative corrections for Ba are roughly of the same magnitude, ranging between about 10 and 120 cm^{-1} for Breit and 15–110 cm^{-1} for the radiative corrections for the levels considered. For the higher levels the radiative corrections dominate.

We see that the deviation of our final results “Total” from experiment, Δ_{Expt} , ranges between 10 and 200 cm^{-1} , with the exception of the larger deviation for $5d^2 \ ^3P_{0,1}$ of about 400 and 500 cm^{-1} and the very large deviation for $5d^2 \ ^1S_0$ of about 1100 cm^{-1} .

The singlet state $5d^2 \ ^1G_4$ has not been measured and is absent in the NIST data [42]. Its position was predicted in the early experimental work of Palenius [46] to be

$24\,300 \pm 300 \text{ cm}^{-1}$. It has subsequently been calculated in Refs. [18,47–49]; there are other calculations of the barium spectra where this level has been missed. We present in the table, alongside our own result, the initial estimate [46] and the value from the most precise calculations [18]. Our calculations give the value 25 205 cm^{-1} for this level; looking at the results for other terms with the configuration $5d^2$, we expect that the result for this level could be underestimated, possibly by as much as 100–300 cm^{-1} .

Our result for $5d^2 \ ^1S_0$ disagrees with the experimental value by $\approx 1100 \text{ cm}^{-1}$. This very large difference is well outside the deviations we see for the other levels. This level does not appear in the extensive spectra calculations of Landau *et al.* [18]. We know of only one other calculation of this level, carried out in the CP+CI method with empirical fitting [20],

TABLE VI. Ionization potentials (removal of one electron, IP1, and both electrons, IP1+IP2) and excitation energies for Ra. CP^{nl}+SD+CI excludes ladder diagrams, Breit, and QED; these corrections are given in subsequent columns. $\Delta_{\text{Expt}} = \text{Total} - \text{Expt}$. Results of other calculations are presented in the final column. Units are in cm^{-1} . Asterisks (*) identify where configurations have been modified from those in the NIST data [42] or where calculated energies in the final column have been reassigned to different terms.

Conf.	Term	J	CP ^{nl} +SD+CI	Ladder	Breit	QED	Total	Expt. ^a	Δ_{Expt}	Other	
IP1	$7s^1$	2S	1/2	42 680	-227	271	-45	42 679	42 573	102	42 622, ^b 42 562 ^c
IP1+IP2	$7s^0$	1S	0	12 4690	-446	250	-132	12 4363	12 4416	-53	12 4656, ^b 12 4642 ^c
$7s7p$	$^3P^o$	0	13 173	-43	70	-64	13 136	13 078	58	12 916, ^b 13 093 ^c	
		1	14 080	-47	71	-64	14 040	13 999	41	13 844, ^b 14 017 ^c	
		2	16 828	-84	78	-60	16 762	16 689	73	16 566, ^b 16 675 ^c	
$7s6d$	3D	1	13 411	380	-46	-92	13 653	13 716	-63	13 622, ^b 14 021 ^c	
		2	13 771	384	-39	-91	14 025	13 994	31	13 902, ^b 14 292 ^c	
		3	14 440	401	-20	-85	14 736	14 707	29	14 645, ^b 14 989 ^c	
$7s6d$	1D	2	16 996	385	-12	-97	17 272	17 081	191	17 004, ^b 17 376 ^c	
$7s7p$	$^1P^o$	1	20 632	-34	69	-61	20 606	20 716	-110	20 667, ^b 20 792 ^c	
$7s8s$	3S	1	26 887	-181	73	-37	26 742	26 754	-12	26 665, ^d 26 762 ^c	
$7s8s$	1S	0	27 910	-119	70	-45	27 816			27 768, ^d 28 248 ^e	
$6d7p$	$^3F^o$	2	27 803	337	26	-161	28 005	28 038	-33	27 991, ^d 28 328 ^c	
		3	29 924	328	46	-155	30 143	30 118	25	30 067, ^d 30 388 ^c	
		4	32 248	303	59	-151	32 459	32 368	91	32 363, ^d 32 603 ^c	
$6d^2$	3F	2	28 964	738	-67	-180	29 455			29 731, ^d 29 610 ^e	
		3	29 648	776	-56	-179	30 189			30 464, ^d 30 404 ^e	
		4	30 455	787	-39	-175	31 028			31 172, ^d 31 114 ^e	
$6d^{2*}$	3P	0	29 426	402	32	-155	29 705			29 840, ^d 29 833 ^e	
		1	30 659	560	10	-164	31 065	31 249	-184	31 365, ^d 31 342 ^e	
		2	31 892	1257	22	-142	33 029	32 941	88	33 180, ^d 33 147 ^e	
$7s8p$	$^1P^o$	1	30 691	51	55	-94	30 703	32 858	-2155	30 695 ^{d*}	
$6d^2$	1D	2	30 490	493	13	-144	30 852			30 982, ^d 30 930 ^e	
$6d7p$	$^1D^o$	2	30 747	312	43	-150	30 952	30 918	34	30 894, ^d 31 178 ^e	
$7s8p$	$^3P^o$	0	31 180	-152	79	-53	31 054	31 086	-32	31 008, ^d 31 126 ^c	
		1	31 511	-5	55	-88	31 473	31 563	-90	31 446, ^{d*} 31 636 ^c	
		2	31 913	-92	75	-64	31 832	31 874	-42	31 778, ^d 31 934 ^c	
$7s7d$	3D	1	32 079	-144	74	-51	31 958	32 001	-43	31 895, ^d 32 423 ^e	
		2	32 749	-810	69	-65	31 943	31 993	-50	31 902 ^d	
		3	32 273	-143	77	-51	32 156	32 197	-41	32 068, ^d 32 625 ^e	
$7s7d^*$	1D	2	32 171	26	53	-84	32 166	32 215	-49	32 205, ^d 32 564 ^e	
$6d7p$	$^3D^o$	1	32 180	-1	52	55	32 136	32 230	-94	32 090, ^d 32 614 ^e	
		2	32 287	279	17	-157	32 426	32 507	-81	32 436, ^d 32 846 ^c	
		3	33 021	254	28	-147	33 156	33 197	-41	33 169, ^d 33 531 ^e	
$6d7p$	$^3P^o$	0	33 543	247	21	-151	33 660	33 782	-122	33 809, ^d 34 055 ^c	
		1	33 586	239	24	-147	33 702	33 824	-122	33 837, ^d 34 102 ^e	
		2	34 193	283	43	-147	34 372	34 383	-11	34 421, ^d 34 677 ^e	
$6d^2$	1G	4	33 142	724	-16	-166	33 684			33 261 ^e	
$6d^2$	1S	0	33 561	312	54	-116	33 811			33 961 ^d	
$6d7p$	$^1F^o$	3	34 230	155	55	-121	34 319			34 332 ^d	
$7s9s$	3S	1	34 601	-224	81	-41	34 417	34 476	-59		

^aNIST data [42].

^bCP+CI [29]. IP1 found in combination with the calculation for the ion [43].

^cXIHFSCC [31]. The value for IP1 includes a QED radiative and frequency-dependent Breit correction of -46 cm^{-1} from Ref. [37].

^dSemiempirical CP+CI [20].

^eIHFSCC [18].

with the result $26 034 \text{ cm}^{-1}$; this is about 700 cm^{-1} less than experiment, and well above the estimated error in that work.

We should note, however, that the largest deviations we see are for terms belonging to $5d^2$, and the unmeasured level $5d^2 \ ^1G_4$ and the level $5d^2 \ ^1S_0$ belong to this configuration. It is possible that our calculations do not do an adequate job for these low-lying d^2 states. We note further the large difference

between our result and that of Ref. [18] for the energy of the level $5d^2 \ ^1G_4$.

The results of the current work are in significantly better agreement with experiment over the considered spectral range compared to the *ab initio* calculations performed using CP+CI [29], SD+CI [32], and a version of Fock-space coupled cluster (FSCC) [45]. There is only one other work where comparable accuracy was reached, using the inter-

TABLE VII. Ionization potentials (removal of one electron, IP1, and both electrons, IP1+IP2) and excitation energies for E120 up to 40 000 cm⁻¹. CP^{nl}+SD+CI excludes ladder diagrams, Breit, and QED; these corrections are given in subsequent columns. Results of other calculations are also presented. Units are in cm⁻¹. Calculated and nonrelativistic *g* factors are given in the final columns.

Conf.	Term	<i>J</i>	CP ^{nl} +SD+CI	Ladder	Breit	QED	Total	CP+CI ^a	FSCC ^b	XIHFSCC ^c	<i>g</i>	<i>g_{NR}</i>	
IP1	8s ¹	² S	1/2	47 702	-510	565	-75	47 682	47 356	47 046	47 089		
IP1+IP2	8s ⁰	¹ S	0	13 7807	-1030	457	-203	13 7031	13 7501	13 6332	13 6920		
8s8p		³ P ^o	0	16 039	-136	123	-90	15 936	15 777	15 328	15 648	0.000	0.000
			1	18 035	-148	125	-92	17 920	17 710	17 382	17 587	1.409	1.500
			2	25 924	-338	153	-88	25 651	25 419	25 308	25 192	1.499	1.500
8s7d		³ D	1	22 904	69	28	-136	22 865	22 985	22 337	22 903	0.500	0.500
			2	23 299	76	42	-134	23 283	23 163	22 494	23 034	1.162	1.167
			3	23 763	96	79	-125	23 813	23 799	23 377	23 782	1.333	1.333
8s8p		¹ P ^o	1	27 827	-331	142	-79	27 559	27 667	28 304	27 513	1.087	1.000
8s7d		¹ D	2	27 666	41	95	-133	27 669	27 438	27 652	27 247	1.006	1.000
8s9s		³ S	1	31 464	-427	145	-63	31 119			30 862	1.998	2.000
8s9s		¹ S	0	32 633	-431	148	-64	32 286				0.000	0.000
8s9p		³ P ^o	0	35 974	-428	159	-75	35 630			35 463	0.000	0.000
			1	36 109	-427	159	-77	35 764			35 595	1.369	1.500
			2	37 908	-462	163	-76	37 533			37 369	1.500	1.500
8s8d		³ D	1	37 880	-427	152	-82	37 523				0.501	0.500
			2	37 932	-426	151	-81	37 576				1.145	1.167
			3	38 094	-424	157	-79	37 748				1.333	1.333
8s9p		¹ P ^o	1	38 131	-457	161	-77	37 758				1.129	1.000
8s8d		¹ D	2	38 341	-417	153	-85	37 992				1.022	1.000
8s10s		³ S	1	39 441	-507	159	-69	39 024				1.999	2.000
8p ² /8s10s		¹ S	0	39 448	-374	180	-112	39 142				0.000	0.000
8p ² /8s10s		¹ S	0	40 137	-341	206	-158	39 844				0.000	0.000
8s7f/8s6f		³ F ^o	2	40 139	-296	167	-104	39 906				0.680	0.667
			3	40 410	-352	168	-77	40 149				1.061	1.083
			4	40 407	-352	168	-76	40 147				1.250	1.250
8s7f/8s6f		¹ F ^o	3	40 255	-333	170	-83	40 009				1.024	1.000

^aReference [29]. IP1 found in combination with the calculation for the ion [43].

^bReference [30].

^cReference [31]. The value for IP1 includes a QED radiative and frequency-dependent Breit correction of -102 cm⁻¹ from Ref. [37].

mediate Hamiltonian Fock-space coupled-cluster (IHFSCC) method [18]; however, in that method the accuracy deteriorates for the higher levels.

We should note that neither Breit nor QED corrections were included in the results of Ref. [29], while QED corrections were not included in those of Refs. [18,32,45]. The QED correction to IP1 was calculated in the work [37] using the radiative potential [36], and the value -19 cm⁻¹ was obtained—the same result we have obtained in this work.

2. Radium

The results for radium are presented in Table VI. It is seen from the table that there are a number of gaps in the experimental data, and accurate theoretical predictions of the missing data are important. We do not agree with all configuration designations used in the experimental data compiled by NIST [42], and we predict that the energy of one of the states (7s8p¹P₁^o) is significantly lower than that given in the data tables, as explained later.

Compared to Ba, the ladder contributions for Ra are smaller for the terms involving *d* orbitals in the dominant configurations, while the contributions to terms from the *ss* and *sp* configurations are larger. The Breit contributions to the excitation energies range from 10 to 81 cm⁻¹ for the levels

considered, while we saw a significantly larger contribution arising from the QED radiative corrections, 37 – 180 cm⁻¹.

Unlike the case with Ba, for Ra the term designations change in some cases when we go from the approximation without ladder diagrams, CP^{nl}+SD+CI, to that with ladder diagrams. This means that it is more difficult to track the changes in energies associated with the ladder corrections, as the terms themselves may differ in these approximations.

The deviations from experiment are generally smaller for Ra than for Ba, with the deviations well under 100 cm⁻¹ for most levels; only a few levels deviate more than 100 cm⁻¹, with the maximum deviation 191 cm⁻¹ for the singlet state 7s6d ¹D₂ (with the exception of 7s8p¹P₁^o, which we address below).

In the final column of Table VI, we list the results of other calculations. For the lower levels, we present the results of *ab initio* calculations, namely, from the CP+CI method [29] and the extended intermediate Hamiltonian Fock-space coupled-cluster (XIHFSCC) method [31]. For the higher levels, where data from these methods are unavailable, we present the results of the IHFSCC method [18] and a semiempirical CP+CI calculation [20]. Both of these calculations miss some of the higher levels that we see. Note that QED corrections to the excitation energies were not taken into account in these other

works [18,29,31], while Breit corrections were also omitted in Ref. [29]. In Ref. [31], the value for IP1 was modified by adding the frequency-dependent Breit and radiative QED corrections from Ref. [37]; the contribution from the radiative corrections, through use of the radiative potential [36], is -42 cm^{-1} , in agreement with the current work. In Ref. [20], while Breit and QED radiative corrections were not included explicitly, these effects were taken into account to some degree through the empirical fitting factors.

The current calculations for radium are the most complete and most accurate to date. With the high accuracy that we have achieved using this method, we can be confident of resolving anomalies with experiment in favor of the theoretical predictions.

The most striking disagreement is with the energy assigned to the state $7s8p^1P_1^0$. In the experimental data [42], the large excitation energy $32\,858\text{ cm}^{-1}$ is given to this state. However, we do not see this level in our calculations; rather, we see a low-lying state, with energy $30\,703\text{ cm}^{-1}$, that is absent in the data. In the relativistic regime, the states are defined by their total angular momentum J and their parity. We see only six levels with $J = 1$ and odd parity in the energy range we have considered, and even extending this range, the next level that we see appears as high as $36\,067\text{ cm}^{-1}$.

As for other supporting theoretical calculations for the $^1P_1^0$ anomaly, results of the semiempirical CP+CI calculation [20] included two levels with $J = 1$ and odd parity with energies $30\,695\text{ cm}^{-1}$ and $31\,446\text{ cm}^{-1}$. These were assigned in that work to the two levels $7s8p^3P_1^0$ and $7s8p^1P_1^0$ in the experimental data, with very large deviations -868 and -1412 cm^{-1} being seen there. We suggest that these calculated excitation energies should instead be assigned to the low-lying levels $7s8p^1P_1^0$ and $7s8p^3P_1^0$. These numbers are in very close agreement with the results of the current work, $30\,703\text{ cm}^{-1}$ and $31\,473\text{ cm}^{-1}$. No data for the corresponding singlet state $^1P_1^0$ were presented in the IHFSCC work [18].

Therefore, we suggest that there is no high-lying singlet state $^1P_1^0$ with energy $32\,858\text{ cm}^{-1}$, though we expect that there should be a lower-lying one with energy around $30\,700\text{ cm}^{-1}$.

We also suggest that configuration assignments for some terms be altered. We do not have any terms in our data with leading configuration $7p^2$ as appears in the experimental data. For the triplet terms $7p^2\ ^3P$, our results indicate instead a strongly dominating configuration $6d^2\ ^3P$. There is also a case where we see that the dominant configuration is $7s7d$ rather than $7p^2$, for the term referred to in the experimental data as $7p^2\ ^1D_2$.

In a system as heavy as radium, and particularly for the higher levels, the validity of the LS system for designating the terms loses much of its meaning. Nevertheless, we still believe that making the previous observations is important, especially when different assignment of the configurations may lead to confusion between the designations of levels.

We note further that with the very strong mixing of configurations in some terms, these designations become less clear, as we have seen for the odd-parity $J = 1$ terms $7s8p^1P_1^0$, $7s8p^3P_1^0$, and $6d7p^3D_1^0$, where the mixing between $7s8p$ and $6d7p$ is very strong.

3. Element 120

Our results for the ionization potentials and excitation energies for E120 are presented in Table VII. We also present the results of our calculations for g factors, and the corresponding nonrelativistic values, to help in identification of the levels. For the higher levels, there is strong mixing between configurations, and we have included the dominant configurations explicitly in the table.

It is seen that the ladder diagrams for E120 are significant, around 400 cm^{-1} for many levels, although the maximum correction for the levels for E120 is less than we saw for the lighter atoms. The d orbitals are well screened by the relativistically contracted s and $p_{1/2}$ orbitals, and there are no low-lying terms with d^2 configuration.

The Breit corrections to the excitation energies are about 150 cm^{-1} for many levels, while the QED radiative corrections are smaller, reaching 158 cm^{-1} in the largest case, for the level $8p^2\ ^1S_0$.

In the final columns we list the results of other *ab initio* calculations: CP+CI [29], a version of FSCC [30], and XIHFSCC [31]. We are also aware of another calculation [38] of the excitation spectra of E120, though the results are so different from all other data (by as much as $10\,000\text{ cm}^{-1}$ for some levels) that we have decided not to present them in the table.

Overall, there is good agreement between the different calculations presented in the table. It should be noted that Breit and QED corrections were not included in the calculations [29], while QED was not included in Refs. [30,31]. Also, there is some sensitivity to the choice of nuclear density. We used the same Fermi distribution that was used in the previous calculation [29], and in that work the volume isotopic shifts were studied; we refer the reader to that work for more details.

The QED radiative correction to the ionization potential IP1 for E120 was calculated recently. Shabaev *et al.* used their model operator approach [50] to calculate the self-energy correction; they obtained -202 cm^{-1} . The total QED correction (including vacuum polarization) was calculated in Ref. [37] using the radiative potential method [36], and they obtained a result of -77 cm^{-1} , in excellent agreement with our own -75 cm^{-1} . Their result is broken down into the self-energy and vacuum polarization contributions, -183 and $+106\text{ cm}^{-1}$, with the former in good agreement with the result of Shabaev *et al.* [50].

The only other calculation of QED corrections to excitation energies for E120 was performed in the work [38]. The corrections were found using the radiative potential method [36] implemented in GRASP [37,39,40], with results in very good agreement with the results of this work.

4. Accuracy

The quality of our calculations can be gauged by comparison of our results with experiment. We found excellent agreement between theory and experiment for barium and radium, $\lesssim 100\text{ cm}^{-1}$ for many cases, and we can expect a similar level in the error for our predictions for E120.

We note that the largest deviations we have seen between theory and experiment mostly involve configurations containing d orbitals. The smaller deviations we see for Ra compared to Ba could be due to the d orbitals being screened (also there are fewer configurations involving d orbitals in the lower levels); this screening effect is even more pronounced for E120, and therefore the associated errors from d orbitals may be reduced.

To further study the limits of our method, particularly in relation to the quality of the correlation potential, we have also performed calculations of the spectra for the three atoms using a different set of screening factors for the Coulomb interaction in the exchange part of the correlation potential. The screening factors were found from the direct diagrams with both electron-electron screening and the hole-particle interaction included; see the second row of Table I. Calculations performed with these modified screening factors gave results that differed from our final results “Total” in Tables V–VII over the full spectral range we considered by about 10–200 cm^{-1} for barium, about 10–100 cm^{-1} for radium, and about 10–200 cm^{-1} for element 120. For E120, the largest deviations occurred for the higher levels corresponding to configurations composed of valence orbitals that are not the lowest for that wave. For many of the levels for Ba and Ra, the results with the adjusted screening factors were better than or as good as the original results (and often on the other side of the experimental values). Therefore,

we estimate an error that is about half the size of these shifts, consistent with the error estimates we obtained by looking at the deviation of the original results from experiment. We expect similar behavior for E120.

IV. CONCLUSION

In summary, we have performed *ab initio* calculations of the spectra of Ba, Ra, and E120 using the recently developed CP+SD+CI method. We have found unprecedented agreement with experiment for Ba and Ra and have made accurate predictions for missing and unreliable data and for the spectra of E120. For Ra, we are confident that the energy assigned to the level $7s8p^1P_1^0$ in the data [42] is incorrect, and we predict a value $\approx 2200 \text{ cm}^{-1}$ smaller. The size of the error for our calculations for Ra is about 100 cm^{-1} or better, while it is slightly larger for Ba. We estimate a similar level of uncertainty for the spectra of E120. Finally, we note that the size of the errors in this *ab initio* method is comparable to the size of the QED radiative corrections.

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