PHYSICAL REVIEW A **78**, 022507 (2008)

Calculations of the spectra of superheavy elements $Z=119$ and $Z=120^{+}$

T. H. Dinh, V. A. Dzuba, V. V. Flambaum, and J. S. M. Ginges
School of Physics, University of New South Wales, Sydney NSW 2052, Australia

(Received 4 June 2008; published 12 August 2008)

High-precision calculations of the energy levels of the superheavy elements $Z=119$ and $Z=120^{+}$ are presented. Dominating correlation corrections beyond the relativistic Hartree-Fock method are included to all orders in the Coulomb interaction using the Feynman diagram technique and the correlation potential method. The Breit interaction and quantum electrodynamics radiative corrections are considered. Also, the volume isotope shift is determined. A similar treatment for Cs, Fr, Ba^{+}, and Ra^{+} is used to gauge the accuracy of the calculations and to refine the *ab initio* results.

DOI: 10.1103/PhysRevA.78.022507 PACS number(s): 32.10.Hq, 31.15.am, 31.30.Gs, 31.30.jf

I. INTRODUCTION

There has been great progress in recent years in the synthesis of superheavy elements (nuclear charge $Z>104$). Elements up to $Z=118$, excluding $Z=117$, have been produced (see, e.g., Refs. [1,2]), and very recently evidence for the naturally occurring element $Z=122$ was reported [3].

Studies of superheavy elements are largely motivated by the predicted "island of stability," which occurs due to the stabilizing nuclear shell effects. Different nuclear models vary in their predictions of the superheavy shell structure (see, e.g., [4]). Experimental investigation of superheavy elements enables one to distinguish between different models.

Experimental efforts are underway to measure the spectra and chemical properties of superheavy elements [5]. A number of theoretical works, from the quantum chemistry and atomic physics communities, have been devoted to these studies (see Refs. in [6,7]).

Leading relativistic effects grow as $(Z\alpha)^2$, where $\alpha=e^2/\hbar c$ is the fine structure constant, and they become very large in superheavy elements. It has been shown that these effects lead to a number of interesting features, such as level inversion in the spectra of some elements (s levels are pulled in and screen the Coulomb potential seen by higher-orbital waves such as d waves, thereby pushing them out) [6].

In the present work we perform relativistic calculations to determine the spectra of the superheavy element $Z=119$ (eka-Fr) and the singly-ionized superheavy element $Z=120$ (eka-Ra^{+}). The isotope with atomic number $Z=120$ and atomic mass number $A=292$ is predicted to be doubly magic in relativistic mean-field nuclear calculations [8].

II. METHOD OF CALCULATION

We perform calculations for Cs, Fr, Ba^{+}, and Ra^{+} to help gauge the accuracy of the calculations for elements 119 and 120^{+} and as a means to reduce the *ab initio* errors for the spectra of these elements through extrapolation.

At the first stage of the calculations we use the relativistic Hartree-Fock (RHF) method. Calculations are performed in the self-consistent potential formed by the $N-1$ electrons in the core (V^{N-1} potential). A complete set of single-electron orbitals is obtained in this way. The orbitals satisfy the equation

$$h_0\psi_0=\epsilon_0\psi_0, \tag{1}$$

where h_0 is the relativistic Hartree-Fock Hamlitonian

$$h_0=c\boldsymbol{\alpha}\cdot\mathbf{p}+(\beta-1)mc^2-\frac{Ze^2}{r}+V^{N-1}. \tag{2}$$

Here $V^{N-1}=V_{\rm dir}+V_{\rm exch}$ is the sum of the direct and exchange Hartree-Fock potentials, N is the number of electrons, $N-1$ is the number of electrons in the closed core, and Z is the nuclear charge.

A. Correlations

The main challenge in calculations of the spectra of superheavy elements is accurate treatment of correlations. We take into account correlations using the correlation potential method [9]. Here, a correlation potential operator Σ is constructed such that its average value for the valence electron coincides with the correlation correction to the energy, $\delta\epsilon_a=\langle a|\Sigma|a\rangle$.

When the single-particle orbitals are found in the Hartree-Fock potential, the many-body perturbation theory expansion for Σ starts in second order in the Coulomb interaction. There are direct and exchange contributions to the correlation potential. Second-order Σ is calculated via direct summation over a discrete set of single-particle orbitals. Rather than working with finite sums and integrals over the real spectrum, we use finite sums over a pseudospectrum. We introduce a cavity of radius $r=40$ a.u. and 40 B splines are used as a basis for the functions.

The *ab initio* calculations may be improved by including three dominating higher-order diagrams into the second-order correlation potential [10]. These are (i) screening of the Coulomb interaction, (ii) the hole-particle interaction in the polarization operator, and (iii) chaining of the correlation potential Σ.

In particular, (i) and (ii) are included into the direct diagrams of Σ using the Feynman diagram technique. For the exchange diagrams we use factors in the second-order Σ to imitate the effects of screening. These factors are $f_0=0.72$, $f_1=0.62$, $f_2=0.83$, $f_3=0.89$, $f_4=0.94$, $f_5=1$; the subscript denotes the multipolarity of the Coulomb interaction. These factors have been estimated from accurate calculations of the higher-order corrections. The chaining of the correlation potential (iii) is included trivially by adding Σ to the Hartree-Fock potential. The energies, with correlations included, are solutions of the equations for the valence electrons,

$$(h_0 + \Sigma)\psi_a = \epsilon_a \psi_a. \tag{3}$$

Further improvements to the wave functions and energies may be made semiempirically through the use of fitting factors f (not to be confused with the Coulomb screening factors above) placed before the correlation potential, i.e.,

$$(h_0 + f\Sigma)\psi'_a = \epsilon'_a \psi'_a. \tag{4}$$

Factors used for element 119 (120^+) are found by fitting to the experimental energies of the lighter electronic analogs Cs and Fr (Ba^+ and Ra^+). The use of fitting factors is considered a means of including effects, such as higher-order correlations, beyond what is included in the *ab initio* approach.

B. Breit interaction

The Breit interaction accounts for magnetic and retardation corrections to the instantaneous Coulomb treatment of the electron-electron interaction. We use the following form for the Breit operator:

$$h^B = -\frac{\boldsymbol{\alpha}_1 \cdot \boldsymbol{\alpha}_2 + (\boldsymbol{\alpha}_1 \cdot \mathbf{n})(\boldsymbol{\alpha}_2 \cdot \mathbf{n})}{2r}, \tag{5}$$

where $\mathbf{r} = \mathbf{n}r$, r is the distance between electrons, and $\boldsymbol{\alpha}$ is the Dirac matrix.

In a similar way to the Coulomb interaction, we determine the self-consistent Hartree-Fock contribution arising from Breit. This is found by solving Eq. (2) in the potential

$$V^{N-1} = V^C + V^B, \tag{6}$$

where V^C is the Coulomb potential and V^B is the Breit potential.

C. Lamb shift

Quantum electrodynamics radiative corrections to the energies (Lamb shifts) are accounted for by use of the radiative potential introduced in Ref. [11]. This potential has the form

$$V_{\mathrm{rad}}(r) = V_U(r) + V_g(r) + V_f(r) + V_l(r), \tag{7}$$

where V_U is the Uehling potential and V_g is the potential arising from the magnetic formfactor. The potential corresponding to the electric form factor is divided into low- and high-frequency parts, respectively,

$$V_l(r) = -\frac{B(Z)}{e} Z^4 \alpha^5 mc^2 e^{-Zr/a_B}, \tag{8}$$

and

$$V_f(r) = -A(Z,r)\frac{\alpha}{\pi}V(r)\int_1^\infty dt \frac{1}{\sqrt{t^2-1}}\left\{\left(1-\frac{1}{2t^2}\right) \times \left[\ln(t^2-1) + 4\ln\left(\frac{1}{Z\alpha}+0.5\right)\right] - \frac{3}{2} + \frac{1}{t^2}\right\}e^{-2trm} \tag{9}$$

where $V(r)$ is the nuclear potential. The coefficient $A(Z,r)$ $=(1.071 - 1.976x^2 - 2.128x^3 + 0.169x^4)mr/(mr + 0.07Z^2\alpha^2)$, where $x = (Z-80)\alpha$, and a_B is the Bohr radius. Equations (8) and (9) were determined semiempirically by fitting to the Lamb shifts of high states of hydrogenlike ions for $Z = 10-110$.

This potential is added to the Hartree-Fock potential,

$$V^{N-1} = V^{N-1} + V_{\mathrm{rad}}. \tag{10}$$

It is included in the self-consistent solution of the core Hartree-Fock states. Core relaxation, demonstrated to be important for the energies of valence p states, is therefore taken into account.

III. RESULTS AND DISCUSSION

We have calculated removal energies for the low-lying states s, $p_{1/2}$, and $p_{3/2}$. Results for Cs, Fr, and element 119 are presented in Table I and those for the ions Ba^+, Ra^+, and 120^+ are presented in Table II. We list results in the RHF approximation and those with correlations included (with dominant diagrams summed to all orders). The *ab initio* results are listed under the column "Σ." In the column to the right, the percentage deviation from experiment is given in brackets. It is seen for Cs, Fr, Ba^+, and Ra^+ that there is excellent agreement with experiment, with disagreement on the order of 0.1%. The largest disagreements are for $7p_{1/2}$ for both Fr (0.5%) and Ra^+ (0.4%).

In the column "$f_{\mathrm{Cs}}\Sigma$" in Table I we list the results for calculations for Fr and element 119 with the factor f_{Cs} found by fitting to the measured energies for Cs. It is clear by looking at the results for Fr that in all cases the results are significantly improved. The deviations from experiment are 0.1% or better. It is the same situation for the results for Ra^+, as can be seen from Table II.

From the trend in the corrections from Cs to Fr, we expect that using fitting factors significantly improves the accuracy of calculations for element 119. Because use of the fitting factors f_{Cs} for Fr calculations leads to such good agreement with experiment, the fitting factors f_{Fr} differ only slightly from f_{Cs}. This means that extrapolation of the spectra for element 119 from Fr gives energies that are only slightly different from those found from extrapolation from Cs. Our final results for element 119 are found using f_{Fr}, presented in Table I. In the final column of Table I we list for element 119 results of another high-precision calculation [19] and postpone discussion of this work until Sec. III B. We see the same pattern for the ions, and our final results for element 120^+ are listed under the column "$f_{\mathrm{Ra}}\Sigma$."

A. Breit and radiative corrections

The results presented in Tables I and II, including our final values, do not explicitly include Breit or radiative corrections. The reason is that all missing corrections (higher-order correlations, Breit and radiative corrections) are accounted for semiempirically by extrapolating from the lighter homologues (see discussion in Sec. III C below). Nevertheless, it is important to understand the size of the Breit and radiative corrections, and this is addressed in this section.

TABLE I. Removal energies for states of Cs, Fr, and element 119 (in units cm^{-1}). f_{Cs}, f_{Fr} are factors placed before Σ, found by fitting to the energies of Cs and Fr, respectively. The numbers in brackets are percentage deviations of the preceding result compared to experiment. In the last column for element 119 we present the results of another high-precision calculation, Ref. [19]. Final values in the present work for element 119 are in column "$f_{\text{Fr}}\Sigma$."

Atom	State	RHF	Σ		$f_{\text{Cs}}\Sigma$		$f_{\text{Fr}}\Sigma$	Expt.[a] or other[b]
Cs	$6s$	27954	31467	(0.2)				31407
	$7s$	12112	12873	(0.0)				12872
	$8s$	6793	7090	(0.0)				7090
	$6p_{1/2}$	18791	20295	(0.3)				20228
	$7p_{1/2}$	9223	9662	(0.2)				9641
	$8p_{1/2}$	5513	5707	(0.2)				5698
	$6p_{3/2}$	18389	19727	(0.3)				19674
	$7p_{3/2}$	9079	9478	(0.2)				9460
	$8p_{3/2}$	5446	5623	(0.1)				5615
Fr	$7s$	28768	32931	(0.2)	32860	(0.0)		32849
	$8s$	12282	13116	(0.1)	13115	(0.0)		13109
	$9s$	6858	7177	(0.0)	7177	(0.0)		7178
	$7p_{1/2}$	18855	20708	(0.5)	20625	(0.1)		20612
	$8p_{1/2}$	9240	9762	(0.3)	9737	(0.0)		9736
	$9p_{1/2}$	5521	5747	(0.3)	5738	(0.1)		5731
	$7p_{3/2}$	17655	18970	(0.2)	18919	(0.0)		18925
	$8p_{3/2}$	8811	9206	(0.2)	9189	(0.0)		9191
	$9p_{3/2}$	5319	5494	(0.2)	5487	(0.1)		5483
Element 119	$8s$	33554	38954		38866		38852	38577
	$9s$	13194	14087		14086		14079	14050
	$10s$	7208	7534		7535		7536	7519
	$8p_{1/2}$	20126	23445		23294		23272	22979
	$9p_{1/2}$	9654	10453		10416		10415	10365
	$10p_{1/2}$	5709	6040		6027		6018	5997
	$8p_{3/2}$	16674	18102		18046		18053	18007
	$9p_{3/2}$	8449	8883		8863		8866	8855
	$10p_{3/2}$	5145	5340		5332		5328	5320

[a] Cs data from Ref. [12] and Fr data from Ref. [13].

[b] Values for element 119 are the results of calculations, Ref. [19].

Breit corrections were calculated in the self-consistent Breit-Hartree-Fock potential and the results are presented in Table III. These numbers should be considered only as an indication of the order of magnitude of the corrections since the correlated Breit corrections may be large. For example, in Ref. [14] it was found for Cs that account of correlations changes the sign for $6s$ (from 3.2 cm^{-1} to -2.6 cm^{-1}). In that work it was found that there is a small suppression due to correlations for $6p_{1/2}$ (7.5 cm^{-1} to 7.1 cm^{-1}) and for $6p_{3/2}$ it is significant (2.9 cm^{-1} to 0.84 cm^{-1}).

Our results for quantum electrodynamics (QED) radiative corrections are listed in Table IV alongside results of other calculations. We are not aware of other data for the ions. As with the Breit corrections, our results should only be considered estimates, to give an idea of the size of these corrections. They are calculated at the Hartree-Fock level, with correlation corrections excluded. (The effect of correlations would be to increase the density of the valence electrons at the nucleus, thereby leading to larger radiative corrections.)

Moreover, the radiative potential itself was found by fitting to states of hydrogenlike atoms for $10 \leqslant Z \leqslant 110$. Due to a lack of data, direct fitting for $Z=119, 120$ was not possible, and it is not clear how well our radiative potential would work in this region.

In Refs. [15,19], ratio methods were used to evaluate the self-energies. In the former they were found from the ratio $E_{\text{se}}\langle V_{\text{vp}}\rangle_{\text{DF}}/E_{\text{vp}}$, where $\langle V_{\text{vp}}\rangle_{\text{DF}}$ is the Uehling potential averaged over Dirac-Fock wave functions for the neutral system, and E_{se} and E_{vp} are self-energy and vacuum polarization (Uehling) corrections to the energies in hydrogenlike systems. In the latter, the ratio is $E_{\text{se}}\langle \nabla U_{\text{nuc}}(r)\rangle_{\text{DF}}/\langle \nabla U_{\text{nuc}}(r)\rangle_{H}$, where U_{nuc} is the nuclear potential and $\langle\ \rangle_H$ denotes averaging over H-like states. In Refs. [16,17] the Lamb shifts are found employing rigorous QED in the field of several different effective atomic potentials. The numbers in the tables give the ranges in the values for the potentials considered. Similarly

TABLE II. Removal energies for levels of Ba$^+$, Ra$^+$, and element 120$^+$ (cm^{-1}). $f_{\rm Ba}$, $f_{\rm Ra}$ are factors placed before Σ, found by fitting to the energies of Ba$^+$ and Ra$^+$, respectively. The numbers in brackets are percentage deviations of the preceding result compared to experiment. Final values for element 120$^+$ are in column "$f_{\rm Ra}\Sigma$."

Atom	State	RHF	Σ		$f_{\rm Ba}\Sigma$		$f_{\rm Ra}\Sigma$	Expt.[a]
Ba$^+$	$6s$	75340	80834	(0.2)				80686
	$7s$	36852	38344	(0.0)				38331
	$8s$	22023	22662	(0.0)				22661
	$6p_{1/2}$	57266	60603	(0.3)				60425
	$7p_{1/2}$	30240	31346	(0.2)				31296
	$8p_{1/2}$	18848	19365	(0.1)				19350
	$6p_{3/2}$	55873	58876	(0.2)				58734
	$7p_{3/2}$	29699	30718	(0.1)				30675
	$8p_{3/2}$	18580	19060	(0.1)				19050
Ra$^+$	$7s$	75899	82034	(0.2)	81871	(0.0)		81842
	$8s$	36861	38454	(0.0)	38440	(0.0)		38437
	$9s$	22005	22677	(0.0)	22675	(0.0)		22677
	$7p_{1/2}$	56878	60743	(0.4)	60535	(0.1)		60491
	$8p_{1/2}$	30053	31297	(0.2)	31241	(0.0)		31236
	$9p_{1/2}$	18748	19322		19306			
	$7p_{3/2}$	52906	55771	(0.2)	55634	(0.0)		55634
	$8p_{3/2}$	28502	29493	(0.1)	29451	(0.0)		29450
	$9p_{3/2}$	17975	18445	(0.1)	18436	(0.0)		18432
Element 120$^+$	$8s$	83168	90145		89964		89931	
	$9s$	38468	40128		40113		40110	
	$10s$	22673	23357		23355		23357	
	$8p_{1/2}$	60027	65430		65141		65080	
	$9p_{1/2}$	31121	32678		32609		32604	
	$10p_{1/2}$	19253	19945		19926		19926[b]	
	$8p_{3/2}$	49295	52003		51873		51874	
	$9p_{3/2}$	27028	27993		27952		27951	
	$10p_{3/2}$	17223	17691		17681		17678	

[a] Ref. [12].

[b] Final result corresponds to fitting from Ba$^+$, since there is no experimental data for Ra$^+$.

to the current work, in Ref. [18] an effective local potential, mimicking self-energy QED effects, is added to the Dirac-Fock potential.

We see good agreement for the "lighter" atoms, though some disagreement for element 119. We already mentioned why our results should be considered as order of magnitude estimates only for the superheavy elements.

We note that in our work, unlike in all other works mentioned, core relaxation is taken into account. This is accomplished by including the radiative potential into the self-consistent procedure for the core. While this effect is relatively small for Cs s levels, it is significant for element 119. For element 119 $8s$, the Lamb shift changes from 85 cm^{-1} to 67 cm^{-1} without and with core relaxation, respectively. For p levels the correction is more dramatic, although the size of the effect itself is much smaller. For element 119 $8p_{1/2}$, we find the radiative correction to the binding energy without and with core relaxation to be 7 cm^{-1} and 1 cm^{-1}. The effect of the core relaxation is to repel the inner electrons (the Lamb shift decreases the binding energy), leading to reduced shielding of the nuclear Coulomb field at small distances where the radiative corrections are determined.

B. Comparison with other calculations

We know of only one other work where high-precision calculations have been performed for spectra of the superheavy elements studied in this work. Eliav *et al.* [19] have performed coupled cluster calculations for element 119 spectra, including both Breit and radiative corrections. The results of their *ab initio* calculations are tabulated alongside our final (semiempirical) values in Table I. We see that generally there is agreement on the level ~0.1%, with larger deviations for $8s$ (0.7%) and $8p_{1/2}$ (1.3%).

We investigated the large deviations for levels $8s$ and $8p_{1/2}$ by calculating the spectra of Cs, Fr, and element 119 with correlations calculated in the second order of perturbation theory ($\Sigma^{(2)}$, with no higher-order screening or hole-particle interactions taken into account). We used fitting fac-

TABLE III. Corrections to removal energies from account of the Breit interaction. n is the principal quantum number of the ground state. Units are cm^{-1}.

State	Cs	Fr	Element 119	Ba^+	Ra^+	Element 120^+
ns	3	6	35	14	26	82
$(n+1)s$	1	2	8	5	10	24
$(n+2)s$	0	1	3	2	5	11
$np_{1/2}$	7	14	34	29	52	112
$(n+1)p_{1/2}$	3	5	11	11	20	41
$(n+2)p_{1/2}$	1	2	5	6	10	20
$np_{3/2}$	3	4	5	12	18	19
$(n+1)p_{3/2}$	1	2	2	5	7	8
$(n+2)p_{3/2}$	0	1	1	3	4	4

tors to mimic higher-order effects, as was done with the full correlation potential Σ, and compared the results to those in Table I. The result for $8s$ obtained in second order from the fit to Cs, $f'_{\text{Cs}}\Sigma^{(2)}_{119}$, differs from that in all orders, $f_{\text{Cs}}\Sigma_{119}$, by 0.3% (more bound) and for $8p_{1/2}$ the difference is -0.3%. With fitting to Fr spectra (using f'_{Fr} and f_{Fr}, respectively, before $\Sigma^{(2)}$ and Σ) the difference is 0.0% for $8s$ and -0.3% for $8p_{1/2}$. For other states, the agreement is -0.1% or better.

For element 120^+, very good agreement for s levels was obtained using the two approaches with fitting to Ba^+ and Ra^+ (0.1% or better). For the p levels, there are larger deviations, the largest being 0.5% for $8p_{1/2}$.

Differences in values for the spectra obtained in the two approaches gives an indication of the error from missed higher-order effects. An estimate of $\sim 0.1\%$ error supports the detailed consideration below.

C. Estimate of the accuracy

Our final results for the superheavy elements do not include either Breit or radiative corrections explicitly and are listed in Tables I and II. The reason is that by using factors obtained by fitting to measured spectra, it appears that some of the Breit and radiative corrections are included.

Let us consider states of Fr and Ra^+ with sizable ($\sim 0.1\%$) Breit and radiative corrections. For Fr this is $7s$. At the *ab initio* level, the deviation from experiment is 0.25% (column "Σ"). With the fitting factor f_{Cs}, the deviation is reduced to a tiny 0.03%. Moreover, the (estimated) contribution from Breit and radiative corrections (Tables III and IV) is much larger than this deviation, being 0.13% of the measured energy. For Ra^+, looking at energies for the states $7s$, $8s$, $7p_{1/2}$, $8p_{1/2}$, it is seen that we have the same story: the

TABLE IV. Radiative corrections to removal energies. Units are cm^{-1}.

Atom	State	This work	Reference [15]	Reference [16]	Reference [17]	Reference [18][a]	Reference [19]
Cs	$6s$	16	15.5	14.9→26.6	12.7→23.1	14.1	18.0
	$7s$	4					4.2
Fr	$7s$	36	38.3	37.1→61.1	23.9→52.6	40.6	28.8
	$8s$	9					2.9
Element 119	$8s$	67	141[b]	140→152		139	83.2
	$9s$	13					22.6
	$8p_{1/2}$	1					18.2
	$8p_{3/2}$	2					3.7
Ba^+	$6s$	37					
	$7s$	12					
Ra^+	$7s$	77					
	$8s$	24					
Element 120^+	$8s$	120					
	$9s$	32					
	$8p_{1/2}$	5					
	$8p_{3/2}$	7					

[a] Self-energies are given in Ref. [18]; we have added vacuum polarization contributions from Ref. [16] calculated at the Dirac-Fock level.

[b] This number is quoted in their later work, Ref. [16], without explanation; in the original work, Ref. [15], the value is 211 in the same units.

value obtained from fitting is everywhere better than the estimated Breit and radiative contributions. This strongly supports the argument that the use of empirical fitting factors takes into account not only the effects of higher-order correlation effects, but also the Breit and radiative corrections to some extent.

The question then becomes, can we expect the same accuracy for element 119 and element 120^+ as has been demonstrated for Fr and Ra^+? Calculations for element 119 and element 120^+ were performed in a similar way as for Fr and Ra^+ and so we expect that extrapolation from the lighter to the heavier systems follows the same pattern we saw from Cs and Ba^+ to Fr and Ra^+. However, when we go to the heavier systems, there is some difference. For instance, the Z dependence of the relativistic, Breit, and radiative corrections for the "light" systems is $\sim Z^2$, while for the superheavy elements this dependence is stronger [15]. It means that extrapolation from Fr to element 119, for instance, is probably not as good as extrapolation from Cs to Fr.

For Cs, Fr, Ba^+, and Ra^+ it is seen that the largest uncertainty in the *ab initio* calculations comes from the unaccounted correlation corrections, these being larger than the estimated Breit and radiative corrections. This is the case for the higher states for element 119 and element 120^+, however, for the ground state these corrections are about the same (0.3% and 0.2%, respectively) [21]. We expect that, as with Fr and Ra^+, use of the empirical fitting factors improves the accuracy of the *ab initio* calculations, and accounts somewhat for Breit and radiative corrections. We expect our calculations for the superheavy elements to be accurate to $\sim$0.1%.

D. Nuclear dependence: Volume isotope shift

For the low s levels of element 119 and element 120^+, we have found that there is a significant dependence on the root-mean-square nuclear charge radius r_{rms}. Our calculations were performed using a two-parameter Fermi distribution for the nuclear density. The values presented in the previous tables were performed with a half-density radius $c=8.0$ fm and 10–90 % width $t=2.0$ fm corresponding to a rms charge radius $r_{\mathrm{rms}}\approx 6.42$ fm. Defining the volume isotope shift in terms of r_{rms},

$$\frac{\delta E}{E} = k\frac{\delta r_{\mathrm{rms}}}{r_{\mathrm{rms}}}, \tag{11}$$

we have found the following values for k for states 8s and 9s for element 119 and element 120^+ at the RHF level:

$$k=-0.0243, \quad \text{element 119 } 8s, \tag{12}$$

$$k=-0.0115, \quad \text{element 119 } 9s, \tag{13}$$

$$k=-0.0180, \quad \text{element } 120^+ \; 8s, \tag{14}$$

$$k=-0.00936, \quad \text{element } 120^+ \; 9s. \tag{15}$$

A table of values for r_{rms} for nuclei $Z=119$ and $Z=120$ calculated in the nuclear Hartree-Fock-BCS approximation can be found in Ref. [20]. The values range from around $r_{\mathrm{rms}}=6.45$ fm to $r_{\mathrm{rms}}=6.95$ fm for the very heavy isotopes. For $r_{\mathrm{rms}}=6.90$ fm, we obtain at the RHF level the value 33 495 cm^{-1} for the removal energy for element 119 8s. The difference between this value and that obtained with $r_{\mathrm{rms}}=6.42$ fm, $\Delta=-59$ cm^{-1}, is comparable to the size of Breit and radiative corrections.

In principle, measurements of the spectra of different isotopes of superheavy elements may be used to get information about nuclear structure.

IV. CONCLUSION

We have performed *ab initio* calculations of removal energies for the the low-lying s and p levels of the superheavy elements $Z=119$ and $Z=120^+$. Semiempirical fitting was used to improve the accuracy of the calculations, accounting for neglected higher-order correlations as well as Breit and radiative corrections. The volume isotope shift was studied. The accuracy of our calculations is estimated to be on the order of 0.1%.

ACKNOWLEDGMENT

This research was supported by the Australian Research Council.

---

[1] S. Hofmann and G. Münzenberg, Rev. Mod. Phys. **72**, 733 (2000).
[2] Y. Oganessian, Phys. Scr., T **T125**, 57 (2006).
[3] A. Marinov *et al.*, e-print arXiv:0804.3869.
[4] M. Bender, P.-H. Heenen, and P.-G. Reinhard, Rev. Mod. Phys. **75**, 121 (2003).
[5] M. Schädel, Angew. Chem., Int. Ed. **45**, 368 (2006).
[6] V. G. Pershina, Chem. Rev. (Washington, D.C.) **96**, 1977 (1996).
[7] E. Eliav, A. Landau, Y. Ishikawa, and U. Kaldor, J. Phys. B **35**, 1693 (2002).
[8] K. Rutz, M. Bender, T. Burvenich, T. Schilling, P. G. Reinhard, J. A. Maruhn, and W. Greiner, Phys. Rev. C **56**, 238 (1997).
[9] V. A. Dzuba, V. V. Flambaum, P. G. Silvestrov, and O. P. Sushkov, J. Phys. B **20**, 1399 (1987).
[10] V. A. Dzuba, V. V. Flambaum, and O. P. Sushkov, Phys. Lett. A **140**, 493 (1989).
[11] V. V. Flambaum and J. S. M. Ginges, Phys. Rev. A **72**, 052115 (2005).
[12] C. E. Moore, *Atomic Energy Levels*, Natl. Bur. Stand. (U.S.) Circ. No. 467 (U.S. GPO, Washington, D.C., 1958), Vol. III.
[13] J. E. Sansonetti, J. Phys. Chem. Ref. Data **36**, 497 (2007).
[14] A. Derevianko, Phys. Rev. A **65**, 012106 (2001).
[15] P. Pyykkö, M. Tokman, and L. N. Labzowsky, Phys. Rev. A

57, R689 (1998).

[16] L. Labzowsky, I. Goidenko, M. Tokman, and P. Pyykkö, Phys. Rev. A **59**, 2707 (1999).

[17] J. Sapirstein and K. T. Cheng, Phys. Rev. A **66**, 042501 (2002).

[18] P. Pyykkö and L.-B. Zhao, J. Phys. B **36**, 1469 (2003).

[19] E. Eliav, M. J. Vilkas, Y. Ishikawa, and U. Kaldor, Chem. Phys. **311**, 163 (2005).

[20] S. Goriely, F. Tondeur, and J. M. Pearson, At. Data Nucl. Data Tables **77**, 311 (2001).

[21] A ballpark error for the *ab initio* correlation calculations is found by looking at the difference of the correlated values with and without fitting.