Study of the ground state of superheavy elements (SHEs) with $120 \leq Z \leq 170$

I.M. Savelyev, M.Y. Kaygorodov, A.V. Malyshev, Y.S. Kozhedub, I.I. Tupitsyn, V.M. Shabaev

May 15, 2024

St. Petersburg State University

Introduction

Method

The relativistic configuration-interaction method in the basis of the Dirac-Fock-Sturm orbitals (CI-DFS).
[I. I. Tupitsyn et al., Phys. Rev. A 68, 022511 (2003); Phys. Rev. A 72, 062503 (2005); Phys. Rev. A 98, 022517 (2018).]

The QED correction within the model-QED-operator approach.
[V. M. Shabaev et al., Phys. Rev. A 88, 012513 (2013); Comput. Phys. Commun. 189, 175 (2015); 223, 69 (2018); A. V. Malyshev et al., Phys. Rev. A 106, 012806 (2022).]

- Excitation energies
- Ionization potentials
- Electron affinities
- Isotope shifts
- X-ray spectrum
- Transition probabilities

Previous studies

1. J. B. Mann and J. T. Waber, The Journal of Chemical Physics 53, 2397 (1970):
    - Dirac-Fock method
    - Breit magnetic interaction by a perturbation method
    - Z up to 131
2. B. Fricke and G. Soff, Atomic Data and Nuclear Data Tables 19, 83 (1977):
    - Dirac-Fock-Slater method
    - no Breit
    - Z up to 173
3. V. I. Nefedov, M. B. Trzhaskovskaya, and V. G. Yarzhemskii, Doklady Physical Chemistry 408, 149 (2006):
    - multiconfiguration Dirac–Fock calculation
    - Breit correction
    - Z up to 164

Aims

1. Studying the influence of QED effects on the ground state of the SHEs within the Dirac-Fock (DF) method
2. Determination of the ground state levels (terms)
3. Taking into account the electron-correlation effects

   Does the one-configuration description remain valid for SHEs?
4. Investigation of the dependence of the ground-state level on how accurately we solve the configuration-interaction (CI) problem

Details of the calculations

Configurations under study

Table 1: The list of the relativistic shells used to generate the relativistic configurations for which the DF-RAV equations are solved.

Z	Core shells	N_{core}	Valence shells
120 – 121	[Rn]$5f\,6d\,7s\,7p_{1/2}$	114	$7p_{3/2}\,8s\,8p_{1/2}\,7d_{3/2}$
122 – 123	[Og]	118	$8s\,8p_{1/2}\,7d_{3/2}\,6f_{5/2}$
124 – 133	[Og]$8s$	120	$8p_{1/2}\,6f_{5/2}\,7d_{3/2}\,5g_{7/2}$
134 – 144	[Og]$8s\,5g_{7/2}$	128	$8p_{1/2}\,6f_{5/2}\,7d_{3/2}\,5g_{9/2}$
145 – 146	[Og]$8s\,8p_{1/2}\,5g_{7/2}$	130	$6f_{5/2}\,7d_{3/2}\,5g_{9/2}\,9s$
147 – 155	[Og]$8s\,8p_{1/2}\,5g$	140	$6f_{5/2}\,7d_{3/2}\,6f_{7/2}\,9s$
156 – 160	[Og]$8s\,8p_{1/2}\,5g\,6f_{5/2}$	146	$6f_{7/2}\,7d_{3/2}\,9s\,7d_{5/2}$
161 – 165	[Og]$8s\,8p_{1/2}\,5g\,6f$	154	$7d_{3/2}\,7d_{5/2}\,9s\,8p_{3/2}$
166 – 168	[Og]$8s\,8p_{1/2}\,5g\,6f\,7d_{3/2}$	158	$7d_{5/2}\,9s\,8p_{3/2}\,9p_{1/2}$
169 – 170	[Og]$8s\,8p_{1/2}\,5g\,6f\,7d$	164	$9s\,8p_{3/2}\,9p_{1/2}\,7f_{5/2}$

Influence of the Breit and QED corrections ($Z = 125$)

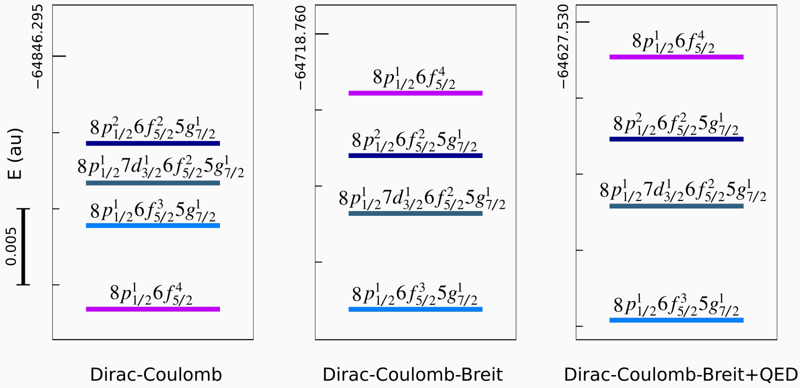

Figure 1: The relativistic-configuration-average energies for the SHEs with $Z = 125$ evaluated using the DF method. The configurations are shown relative to the closed-shell one [Og]$8s^2_{1/2}$.

Level structure

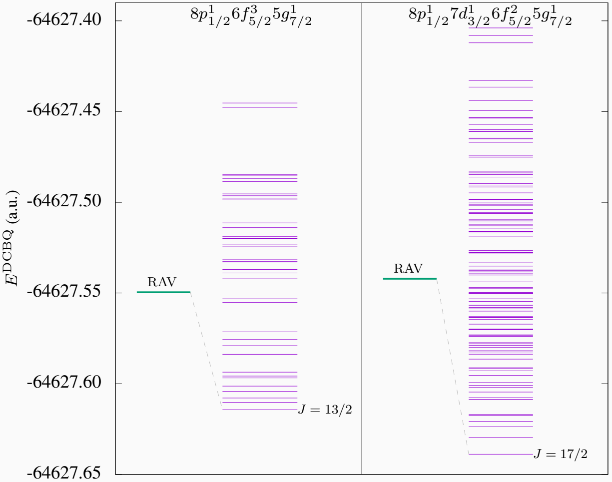

Figure 2: Relativistic-configuration-average energies $E^{\mathrm{DCBQ}}_{\mathrm{RAV}}$ calculated for the configurations $8p^1_{1/2}6f^3_{5/2}5g^1_{7/2}$ (left) and $8p^1_{1/2}7d^1_{3/2}6f^2_{5/2}5g^1_{7/2}$ (right) of the SHE with $Z = 125$ and all the levels which contribute to these energies.

Rearrangements

Table 2: The levels with lowest total energies, the main configurations contributing to them, and the total angular momenta J evaluated by means of the Dirac-Fock and Configuration-interaction schemes.

Z	Dirac-Fock	J_{DF}	Configuration-interaction	J_{CI}
124	$8p^1_{1/2}7d^1_{3/2}6f^2_{5/2}$	6	$0.83 \times 8p^1_{1/2}6f^3_{5/2}$	5
133	$8p^1_{1/2}7d^1_{3/2}6f^3_{5/2}5g^8_{7/2}$	13/2	$0.87 \times 8p^2_{1/2}6f^3_{5/2}5g^8_{7/2}$	9/2
143	$7d^2_{3/2}6f^3_{5/2}5g^8_{9/2}$	5/2	$0.93 \times 7d^2_{3/2}6f^3_{5/2}5g^8_{9/2}$	3/2
155	$7d^2_{3/2}6f^7_{7/2}$	7/2	$0.99 \times 9s^1_{1/2}6f^8_{7/2}$	1/2
167	$9s^1_{1/2}8p^1_{3/2}9p^1_{1/2}$	3/2	$0.88 \times 9s^2_{1/2}8p^1_{3/2}$	3/2

Results

CI results

Z	$8s$	$5g_{7/2}$	$5g_{9/2}$	$6f_{5/2}$	$6f_{7/2}$	$7d_{3/2}$	$7d_{5/2}$	$8p_{1/2}$	$8p_{3/2}$	$9s$	$9p_{1/2}$
119	1										
120	2										
121	2							1			
122	2					1		1			
123	2			1		1		1			
124	2			3				1			
125	2	1		2		1		1			
126	2	2		2		1		1			
127	2	3		2		1		1			
128	2	4		2		1		1			
129	2	4		3		1		1			
130	2	5		3				2			
131	2	6		3				2			
132	2	7		3				2			
133	2	8		3				2			
134	2	8		4				2			
135	2	8	1	4				2			
136	2	8	2	3		1		2			
137	2	8	3	3		1		2			
138	2	8	4	3		1		2			
139	2	8	5	3		1		2			
140	2	8	6	3		1		2			
141	2	8	7	2		2		2			
142	2	8	8	2		2		2			
143	2	8	8	3		2		2			
144	2	8	9	3		2		2			

Figure 3: The main contribution to the ground-state configurations of the superheavy elements by means of the CI method (borrowed from [O. Smits et al., Nature Reviews Physics, 6(2), 86-98 (2024)]).

Z	$8s$	$5g_{7/2}$	$5g_{9/2}$	$6f_{5/2}$	$6f_{7/2}$	$7d_{3/2}$	$7d_{5/2}$	$8p_{1/2}$	$8p_{3/2}$	$9s$	$9p_{1/2}$
145	2	8	10	3		2		2			
146	2	8	10	4		2		2			
147	2	8	10	5		2		2			
148	2	8	10	6		2		2			
149	2	8	10	6		3		2			
150	2	8	10	6	1	3		2			
151	2	8	10	6	2	3		2			
152	2	8	10	6	4	2		2			
153	2	8	10	6	5	2		2			
154	2	8	10	6	6	2		2			
155	2	8	10	6	8			2		1	
156	2	8	10	6	8	2		2			
157	2	8	10	6	8	3		2			
158	2	8	10	6	8	4		2			
159	2	8	10	6	8	4		2		1	
160	2	8	10	6	8	4	1	2		1	
161	2	8	10	6	8	4	2	2		1	
162	2	8	10	6	8	4	3	2		1	
163	2	8	10	6	8	4	5	2			
164	2	8	10	6	8	4	6	2			
165	2	8	10	6	8	4	6	2		1	
166	2	8	10	6	8	4	6	2		2	
167	2	8	10	6	8	4	6	2	1	2	
168	2	8	10	6	8	4	6	2	1	2	1
169	2	8	10	6	8	4	6	2	2	2	1
170	2	8	10	6	8	4	6	2	2	2	2

Figure 4: The main contribution to the ground-state configurations of the superheavy elements by means of the CI method (borrowed from [O. Smits et al., Nature Reviews Physics, 6(2), 86-98 (2024)]).

The periodic table of the elements

Period	s 1	2	3	d 4	5	6	7	8	9	10	11	12	p 13	14	15	16	17	18	
6	55 Cs	56 Ba	57–71	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn	6*s*5*d*6*p*
7	87 Fr	88 Ra	89–103	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Nh	114 Fl	115 Mc	116 Lv	117 Ts	118 Og	7*s*6*d*7*p*
8	119	120	125–155	156	157	158/159	160	161	162		163	164			167				8*s*7*d*8*p*
9	165	166											169	170					9*s*9*p*

6	57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu	4*f*
7	89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr	5*f*
8			145	146	147	148/149	150	151		152	153	154		155		6*f*

8	125	126	127	128/129	130	131	312	133/134	135	136	137	138	139	140	141	142/143	144	145	5*g*

Figure 5: An attempt to place the superheavy elements into the PTE (borrowed from [O. Smits et al., Nature Reviews Physics, 6(2), 86-98 (2024)]).

For more details: I. M. Savelyev et al., Phys. Rev. A 107, 042803 (2023).