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Electronic Configurations and the Periodic Table
for Superheavy Elements

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The periodicity of the chemical properties of elements is associated with the repetition of the configurations of valence electrons with respect to the quantum number *l*, which dictates the angular distribution of wave functions in the nonrelativistic approximation and, thus, determines the chemical properties. However, for superheavy elements ($Z > 111$), which have been successfully synthesized in the last years [1–4], relativistic effects are crucial and lead to a noticeable violation of simple regularities [5, 6]. In early works on the electronic configurations of superheavy elements [5–7], configuration interaction was not considered and some calculations were performed by the Dirac–Fock–Slater method with approximate inclusion of exchange, which is less accurate than the Dirac–Fock method.

In this work, we performed multiconfiguration Dirac–Fock calculations with inclusion of the total angular momentum coupling scheme and the Breit correction. The lowest lying term was taken to be the energy of a given configuration. When these energies for different configurations were very close to one another, configuration interaction was included in the calculations [8]. The calculations covered the elements with $119 \leq Z \leq 164$. Configuration interaction calculations were necessary since the total energies of different configurations differ little from one another in many cases [5]. Therefore, inclusion of configuration interaction can lead to a change of the ground-state configuration. In particular, it is worth noting that about one half of the ground-state configurations obtained in this work differ from those reported in [7], where no configuration interaction was included and the exchange energy was considered by an approximate statistical method. Dirac–Fock calculations were performed for many heavy elements [9], but configuration interaction was not included. These data are compared with our data in Tables 1 and 2. This comparison shows that configuration interaction is crucial in more than 30% of cases

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since its consideration leads to another ground-state configuration. The calculated electronic configurations of some elements (up to $Z = 120$) were reported in [10–14].

Table 1. Ground-state configurations of atoms with $119 \leq Z \leq 145$

Atomic number Z	Electronic shells	
	this work	[9]
119	$8s$	$8s$
120	$8s^2$	$8s^2$
121	$8s^2 8p$	$8s^2 8p$
122	$7d8p$	$7d8p$
123	$6f^2 8p$	$6f7d8p$
124	$6f^2 8p^2$	$6f^3 8p$
125	$0.81(5g6f^2 8p^2) + 0.17(5g6f7d^2 8p)$ $+ 0.02(6f^3 7d8p)$	$5g6f^3 8p$
126	$0.998(5g^2 6f^3 8p) + 0.002(5g^2 6f^2 8p^2)$	$5g^2 6f^2 7d8p$
127	$0.88(5g^3 6f^2 8p^2) + 0.12(5g^3 6f7d^2 8p)$	$5g^3 6f^2 8p^2$
128	$0.88(5g^4 6f^2 8p^2) + 0.12(5g^4 6f7d^2 8p)$	$5g^4 6f^2 8p^2$
129	$5g^4 6f^3 7d8p$	$5g^5 6f^2 8p^2$
130	$5g^5 6f^3 7d8p$	$5g^6 6f^2 8p^2$
131	$0.86(5g^6 6f^3 8p^2) + 0.14(5g^6 6f^2 7d^2 8p)$	$5g^7 6f^2 8p^2$
132	$5g^7 6f^3 8p^2$	$5g^8 6f^2 8p^2$
133	$5g^8 6f^3 8p^2$	$5g^8 6f^3 8p^2$
134	$5g^8 6f^4 8p^2$	$5g^8 6f^4 8p^2$
135	$5g^9 6f^4 8p^2$	$5g^9 6f^4 8p^2$
136	$5g^{10} 6f^4 8p^2$	$5g^{10} 6f^4 8p^2$
137	$5g^{11} 6f^4 8p^2$	$5g^{11} 6f^3 7d8p^2$
138	$5g^{12} 6f^3 7d8p^2$	$5g^{12} 6f^3 7d8p^2$
139	$5g^{13} 6f^3 7d8p^2$	$5g^{13} 6f^3 7d8p^2$
140	$5g^{14} 6f^3 7d8p^2$	$5g^{14} 6f^3 7d8p^2$
141	$5g^{15} 6f^2 7d8p^2$	$5g^{15} 6f^2 7d^2 8p^2$
142	$5g^{16} 6f^2 7d8p^2$	$5g^{16} 6f^2 7d^2 8p^2$
143	$5g^{17} 6f^2 7d8p^2$	$5g^{17} 6f^2 7d^2 8p^2$
144	$0.95(5g^{17} 6f^2 7d^3 8p^2)$ $+ 0.05(5g^{17} 6f^4 7d8p^2)$	$5g^{18} 6f7d^3 8p^2$
145	$5g^{18} 6f^3 7d8p^2$	$5g^{18} 6f^3 7d^2 8p^2$

Table 2. Ground-state configurations of atoms with $146 \leq Z \leq 164$

Atomic number Z	Electronic shells	
	this work	[9]
146	$6f^4 7d^2 8p^2$	$6f^4 7d^2 8p^2$
147	$6f^5 7d^2 8p^2$	$6f^5 7d^2 8p^2$
148	$6f^6 7d^2 8p^2$	$6f^6 7d^2 8p^2$
149	$6f^6 7d^3 8p^2$	$6f^6 7d^3 8p^2$
150	$6f^7 7d^3 8p^2$	$6f^6 7d^4 8p^2$
151	$6f^8 7d^3 8p^2$	$6f^8 7d^3 8p^2$
152	$6f^9 7d^3 8p^2$	$6f^9 7d^3 8p^2$
153	$6f^{10} 7d^3 8p^2$	$6f^{11} 7d^2 8p^2$
154	$6f^{11} 7d^3 8p^2$	$6f^{12} 7d^2 8p^2$
155	$6f^{12} 7d^3 8p^2$	$6f^{13} 7d^2 8p^2$
156	$6f^{13} 7d^3 8p^2$	$6f^{14} 7d^2 8p^2$
157	$6f^{14} 7d^3 8p^2$	$6f^{14} 7d^3 8p^2$
158	$6f^{14} 7d^4 8p^2$	$6f^{14} 7d^4 8p^2$
159	$6f^{14} 7d^4 8p^2 9s^1$	$6f^{14} 7d^4 8p^2 9s^1$
160	$6f^{14} 7d^5 8p^2 9s^1$	$6f^{14} 7d^5 8p^2 9s^1$
161	$6f^{14} 7d^6 8p^2 9s^1$	$6f^{14} 7d^6 8p^2 9s^1$
162	$6f^{14} 7d^7 8p^2 9s^1$	$6f^{14} 7d^8 8p^2$
163	$6f^{14} 7d^8 8p^2 9s^1$	$6f^{14} 7d^9 8p^2$
164	$6f^{14} 7d^{10} 8p^2$	$6f^{14} 7d^{10} 8p^2$

Table 3. Average radii $\langle R \rangle$ (au) of electron wavefunctions for the element with $Z = 130$

Shell	$\langle R \rangle$	Shell	$\langle R \rangle$
$5g_{7/2}$	0.641	$7p_{1/2}$	1.386
$6s$	0.637	$6f_{5/2}$	1.614
$6p_{1/2}$	0.650	$7d_{3/2}$	3.268
$6d_{3/2}$	0.987	$8s$	3.267
$7s$	1.300	$8p_{1/2}$	3.974

The ground-state electronic configurations of superheavy elements are summarized in Tables 1 and 2. These data allow us to draw the following conclusions.

Elements 119, 120, and 121 are analogues of Fr, Ra, and Tl, respectively. The elements beginning with element 122 have no analogues in the upper part of the periodic table, and the 5g electronic shell begins to fill at $Z = 125$. Elements 121–157 can be classified as the period of 5g and 6f electrons. In principle, two sequences of elements can be considered: the elements from 122 to 145 form the period of 5g electrons, and the elements from 145 to 157 form the period of 6f electrons. However, the 6f states start filling up even at $Z = 123$. In addition, all elements from 122 to 157 have some features in common.

Indeed, both the 5g and the 6f electrons are not involved in covalent bonding since the average radii of the 5g and 6f wavefunctions are closer to the average radii of the 6s, 6p, 6d, 7s, and 7p inner shells than to the average radii of the 8s, 8p, and 7d valence shells (Table 3). As a result, these elements should be characterized by relatively low oxidation states determined by the presence of the 8s, 8p, and 7d electrons. Higher oxidation states exceeding the total number of the 8s, 8p, and 7d electrons, obviously, cannot be ruled out, but these compounds should be rather strong oxidants.

The figure shows a fragment of the periodic table for superheavy elements constructed taking into account the electronic configurations obtained. For the sake of economy of space, the short-form periodic table is shown. It is worth noting that the period of the 5g and 6f elements begins in Group III (in the short-form periodic table), just as takes place for lanthanides and actinides. However, for lanthanides (4f elements) and actinides (5f elements), the first elements of these series, La and Ac, are analogues of Y, i.e., of a d element. For the series of the 5g and 6f elements, the first element, with $Z = 121$, is an analogue of Tl, i.e., of a p element. It is hard to decide whether this is due to the change of parity ($f \rightarrow d$ and $g \rightarrow p$) or is accidental. When the 5g and 6f shells are complete ($Z = 157$), the 7d shell should successively fill beginning with element 158. This is actually the case (Table 2). Element 164 has the complete 7d shell.

It is worth noting that, as distinct from the 5p elements, d elements belonging to the same group of the periodic table do not always have the same electronic configuration. For example, the electronic configurations of Ni, Pd, and Pt are $3d^8 4s^2$, $4d^{10}$, and $5d^9 s$, respectively. The number of such examples can be easily increased. The electronic configurations of elements 158–164 are rather close to those of their 4d congeners Zr ($d^2 s^2$), Nb ($d^4 s$), Mo ($d^5 s$), Tc ($d^5 s^2$), Ru ($d^7 s$), Rh ($d^8 s$), and Pd (d^{10}) (see the data for elements 158–164 in Table 2). In principle, the contradiction consisting of the fact that elements placed one under another in a group have different electronic configurations and, hence, different chemical properties can be removed if the periodic table is presented in a three-dimensional form. This is true, for example, for elements 111 (Rg) and 112, whose configurations differ significantly from those of Au and Hg, placed in the same groups (see [5] for details). In the three-dimensional representation of the periodic table, elements 111 (Rg) and 112 can be displaced from the plane in which Au and Hg and their analogues are located (figure). The same procedure can be applied to other similar cases. Thus, it can be readily shown why high-spin tetrahedral compounds are typical of Ni and not typical of Pd and Pt. It is not worth-

6	Cs	Ba	La–Lu*	Hf	Ta	W	Re	Os	Ir	Pt
	Au	Hg	Tl	Pb	Bi	Po	At	Rn		
7	Fr	Ra	Ac–Lr**	Rf	Db	Sg	Bh	Hs	Mt	Ds
	Rg	112	113	114	115	116	117	118		
8	119	120	121–157***	158	159	160	161	162	163	164

Fragment of the periodic table for heavy and superheavy elements: * lanthanides, ** actinides, and *** the period of the 5*g* and 6*f* elements.

while to try to reflect the whole range of chemical properties of elements of the same group in one such table; however, the three-dimensional periodic table calls attention to this problem. It should be taken into account that a difference in the chemical properties of elements of the same group can be not only due to a difference in their electronic structure but also due to different shielding of valence electrons.

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