

A suggested Periodic Table up to $Z \leq 172$, based on Dirac-Fock calculations on atoms and ions[†]

Pekka Pyykkö^{*a}

Received Xth XXXXXXXXXXXX 20XX, Accepted Xth XXXXXXXXXXXX 20XX

First published on the web Xth XXXXXXXXXXXX 200X

DOI: 10.1039/b000000x

Extended Average Level (EAL) Dirac-Fock calculations on atoms and ions agree with earlier work in that a rough shell-filling order for the elements 119-172 is $8s < 5g \leq 8p_{1/2} < 6f < 7d < 9s < 9p_{1/2} < 8p_{3/2}$. The present Periodic Table develops further that of Fricke, Greiner and Waber [*Theor. Chim. Acta* 1971, **21**, 235] by formally assigning the elements 121-164 to (nlj) slots on the basis of the electron configurations of their ions. Simple estimates are made for likely maximum oxidation states, i , of these elements M in their MX_i compounds, such as $i = 6$ for UF_6 . Particularly high i are predicted for the 6f elements.

1 Introduction

The Periodic Table (PT) is a compact, approximate way to summarise both the electronic shell structure of individual atoms, or their ions, and chosen aspects of the chemical behaviour of the elements. The history of the PT was recently discussed by Kaji¹, Gordin² and Scerri³. We also quote the study on certain (n, l) ('Madelung') rules by Ostrovsky⁴ and the attempts at a group-theoretical classification of the elements by Kibler⁵. The underlying electronic principles were discussed by Schwarz et al.⁶⁻⁸.

A modern, 18-column, shape of the PT is shown in Figure 1. The latest two essential additions were the addition of the 5f or actinide elements by Seaborg (see¹⁰) and the now completed transactinide series up to $Z = 118$. The last of them was the case $Z = 117$, reported in 2010 by Oganessian et al.¹¹. One often speaks of 'Superheavy Elements (SHE)'. Chemically speaking, decades of both experimental¹²⁻¹⁴ and theoretical^{15,16} work give good reason to regard at least the elements 104-109 as a fourth, 6d transition-metal series. A drastic change of the covalent radii may occur from E110 (Darmstadtium, Ds) onwards, see Figure 2. The experimental chemical studies on the elements $Z \leq 118$, and maybe beyond, are of the type 'one atom at a time'. In cases where the nuclear lifetimes now are too short for chemical studies, new, more neutron-rich isotopes may help. Studies on the bulk chemistry are expected to remain computational, only.

The values $l = 0, 1, 2, 3, 4$ are denoted by the symbols s, p, d, f, g respectively. When necessary, the lower spin-orbit (SO) split component $j = l - \frac{1}{2}$ is denoted by a star, $e.g.$ $p^* = p_{1/2}$. The principal quantum number n of the s and

Period	Periodic Table 1-118																18 Orbitals		
1	1 H	2 He											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar	1s
2	3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne	2s2p
3	11 Na	12 Mg	3	4	5	6	7	8	9	10	11	12	13 Al	14 Si	15 P	16 S	17 Cl	18 Ar	3s3p
4	19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr	4s3d4p
5	37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe	5s4d5p
6	55 Cs	56 Ba	57-71 La	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	6s5d6p
7	87 Fr	88 Ra	89-103 Ac	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113	114	115	116	117	118	7s6d7p
8	101 La	102 Ce	103 Pr	104 Nd	105 Pm	106 Sm	107 Eu	108 Gd	109 Tb	110 Dy	111 Ho	112 Er	113 Tm	114 Yb	115 Lu				4f
9	109 Ac	110 Th	111 Pa	112 U	113 Np	114 Pu	115 Am	116 Cm	117 Bk	118 Cf	119 Es	120 Fm	121 Md	122 No	123 Lr				5f

Fig. 1 The Periodic Table of the 118 experimentally known elements. The numbers $g = 1 - 18$ are the Groups. The IUPAC PT⁹ coincides with this table, but so far only includes the elements, up to Rg.

p shells coincides with the number of the period in Figure 1. It should be stressed that, while nuclear charges are well defined, the concept of an electron configuration, both for atoms and molecules, is only approximate. For both systems, the true many-electron wave function can be a superposition of a large number of effective electron configurations. This aspect especially affects the transition metals.

The filling of such shells up to $Z = 172$ was studied using Dirac-Slater (DS) theory by Fricke et al.^{19,20} for single, jj -coupled electron configurations in this approximate form of density functional theory (DFT). It was found that, approximately for $Z = 121-143$, $8p_{1/2}$ and $5g$ shells become occupied in neutral atoms. The full 6f and 7d series are completed

^a Department of Chemistry, University of Helsinki, POB 55 (A. I. Virtasen aukio 1), FI-00014 Helsinki, Finland. Fax: +358 9 19150169. E-mail: Pekka.Pyykko@helsinki.fi

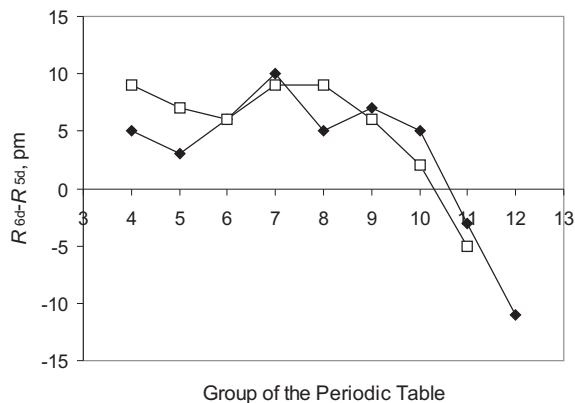


Fig. 2 The collapse after Group 10 of the 7th Period ('6d') covalent radii, compared to 6th-Period ('5d') ones. Black diamonds: Single-bond radii¹⁷. Open squares: Triple-bond radii¹⁸.

around $Z = 144-154$ and $155-164$, respectively. The following row contained the $9s$, $9p_{1/2}$ and $8p_{3/2}$ elements $165-166$, $167-168$ and $169-172$, respectively, see Figure 10 of ref.¹⁹. The heaviest atom treated seems to be $E184$ ²¹. The primary, numerical DS data are listed in ref.²².

Already slightly earlier, Waber^{23,24} found $5g$ electrons in the atomic ground state from $E125$ on. Lu et al.²⁵ also provided DS data up to $Z=126$. At Dirac-Fock (DF) level, Mann²⁶ noticed the particular stability of the $8p^*$ shell and Mann and Waber²⁷ reported results for $E118-E131$. The general conclusion is that, around $E121-131$, both $8p$, $7d$, $6f$ and $5g$ orbitals may enter the atomic ground states.

At this point one should point out that a realistic finite nuclear size keeps the lowest ($1s$) eigenvalue within the normally allowed range $\epsilon > -2mc^2$ (a free electron being taken as $\epsilon = 0$). For the $1s$ state of a one-electron atom, and the available nuclear models, the critical limit, Z_{cr} has been put at $Z = 175$ ²⁸, >170 ²⁹ or 171.5 ³⁰. The screening from the other electrons should raise that limit.

Zel'dovich and Popov^{31,32} actually point out that the electron wave functions remain localized beyond Z_{cr} but this behaviour has not been implemented in any atomic codes yet.

It is not obvious how to treat the quantum electrodynamical (QED) effects in the supercritical domain $Z > 137$. Here they are hence simply dropped out. In the range $Z = 50-100$, they are typically -1% of the one-electron, Dirac-level relativistic effects³³⁻³⁵, on the valence ns orbital binding energies of neutral or nearly neutral atoms. For a recent summary on the QED aspects, see Indelicato et al.³⁶. Because their sign on s levels is repulsive, they should also increase Z_{cr} .

Average-of-configurations Dirac-Fock (DF) calculations for the elements $1-120$ were reported by Desclaux³⁷. Ume-

moto and Saito³⁸ also found $5g$ electrons to appear at $E126$ at DS level. Very precise relativistic coupled-cluster calculations were reported by the group of Kaldor on individual atoms and their ions, such as $E122$ ³⁹. Multiconfiguration, MCDf-level calculations on the atomic ground configurations for elements $119-164$ were reported by Nefedov et al.⁴⁰ who, however, do not specify the exact computational method used, nor the value of the total atomic angular momentum, J .

Little molecular work has been done on superheavy elements beyond the rare gas $E118$ (which has an electron affinity^{41,42}). The exceptions comprise an MS $X\alpha$ study of $5g^1$ complexes of $E125$ ⁴³ (entirely supporting the present PT), a single-configuration DF study on diatomic $(E126)F$ ⁴⁴ and a study on $(E119)H$ and $(E120)H^+$ ⁴⁵.

The purpose of present work is to extend the previous work on neutral atoms to chemically plausible ions, fully realising the difference between free ions and ions in chemical compounds, at a - still approximate - but realistic DF level, in order to see how a 21st-Century Periodic Table could possibly be shaped in its most compact, approximate form.‡

2 Methods

The calculations were performed using the latest version of the MCDf program of Desclaux and Indelicato⁴⁶, at the Extended Average Level (EAL) level. Because many atomic levels can be mixed in chemical-bond formation, as emphasized by Schwarz and coworkers⁶, this may actually be a desirable approximation. The EAL is useful, as long as the spin-orbit (SO) effects are not excessive, or can be separately checked.

The nuclear charge distribution was taken as a Fermi one with the parameters

$$\rho(r) = \rho_0 / [1 + \exp((r-c)(4 \ln 3)/t)], \quad (1)$$

where ρ_0 is a normalization constant to obtain a charge Z and the surface thickness $t = 2.3$ fm (Fermi) for $Z > 45$. Using

$$A = 0.00733Z^2 + 1.3Z + 63.6. \quad (2)$$

for the atomic mass, the RMS nuclear radius c (in fm) is extrapolated in the program from known values of c as a function of $A(Z)$ for large Z . We have not studied here the chemical effects of varying the nuclear size.

Some calibration results are compared to earlier ones in the Table 1.

‡ The present work was done in preparation for a lecture at the 150th Anniversary Congress of "Weltkongress Chemie" in 1860 at Karlsruhe on 3-4 September, 2010.

Table 1 Comparisons of the present EAL results against literature. PW = present work.

Z	q	El. conf.	$2J$	$I/a.u.$	Reference
121	0	$8p^1$	1	0.113 0.1634	PW 47
	+1	$8s^2$	0	0.423 0.4652	PW 47
	+2	$8s^1$	1	0.653 0.6854	PW 47
	+3	$8s^0$	0	1.627	PW
	+4	$7p^{-1}$			PW
122	0	$8s^2 8p 7d$	4	0.206	39
	+1	$8s^2 7d$	3	0.415	39
	+2	$8s^2$	0	0.704 0.749	PW 39
	+3	$8s^1$	1	0.961 0.997	PW 39

3 Results

3.1 A broad mapping

A compact, very schematic grouping of the elements up to $Z = 172$ is shown in Figure 3. The underlying atomic results are shown in Tables 2 and 3.

3.2 Elements 119-126 and the beginning of a 5g series

As discussed before, elements 119 and 120 are $8s^1$ and $8s^2$, and thus belong to Groups 1 and 2, respectively^{19,37,48,49}. For neutral E121, the present EAL calculations prefer $8p$, with $7d$ only slightly above. The one-electron ions E123⁴⁺ and E124⁵⁺ switch the $8s$ ground state for a $6f$. From E125⁶⁺ onwards, a $5g^1$ state is preferred, as seen in Table 2. The one-electron ions E125⁶⁺ and E126⁷⁺ being clearly $5g^1$, this motivates placing these elements in Groups 7 and 8, of a beginning 5g row, respectively. A chemical example on the former would be the (E125)F₆ of Makhyoun⁴³. For the next element, the (E126)F₆ are then expected to be $5g^2$ systems. An analog for the one-electron ions is Ce³⁺, $4f^1$, placed in Group 4. Further analogs are U⁵⁺ and Np⁶⁺, both $5f^1$, placed in Groups 6 and 7, respectively. There is room for 18 elements E121-E138 on this 5g row. We repeat that we do not mind if other orbitals, such as $8p^*$, $7d$, or $6f$ ones could be occupied in some early members of a row, or in low oxidation states of these elements. They are nevertheless counted as members of the 5g series.

Note that, depending on the oxidation state, the $8s$ occupation may vary from 0 to 2. In this sense the $8s$ and $5g$ levels cross. Concerning the filling of the $5g$ shell, in the neutral-atom calculations, this does not occur until E144¹⁹.

The size of the $5g$ orbitals being very small (see Section 4), their direct involvement in chemical bonding is unlikely, just

as in the case of the $4f$ orbitals of the lanthanides.

Table 2 Calculated electron configurations for nuclear charge Z and ionicity q for $Z \leq 140$. The post-E118 electron configuration is shown. The quantity I is the energy of the next ionization. Further data for E121 and E122 are given in Table 1. An 'r' in the last column indicates that the corresponding r_{\max} was included in Figure 4 below.

Z	q	El. conf.	$I/a.u.$	Exc. en.	
119	0	$8s^1$			r
120	0	$8s^2$			r
121	0	$8s^2 8p^1$	0.113		r
		$8s^2 7d^1$		+0.0042	r
	+1	$8s^2$			
123	+4	$6f^1$	1.374		r
124	+5	$6f^1$	1.918		r
		$5g^1$		+0.0948	r
125	+6	$5g^1$	2.721		r
	+7	$5g^0$			
126	+6	$5g^2$	2.714		r
		$6f^1 5g^1$		+0.2091	r
	+7	$5g^1$	3.677		
133	+6	$5g^9$			r
136	+2	$8s^2 6f^3 5g^{11}$			
	+6	$5g^{12}$			
138	+5	$8s^2 5g^{13}$	2.089		
		$8s^1 5g^{14}$		+0.0977	
		$6f^2 5g^{13}$		+0.2146	
		$6f^1 5g^{14}$		+0.2923	
		$6f^3 5g^{12}$		+0.3779	
		$8p^1 5g^{14}$		+0.7159	
		$8s^1 5g^{13}$			r
		$6f^1 5g^{13}$		+0.0225	
		$5g^{14}$		+0.0360	
		$6f^2 5g^{12}$		+0.2509	
140	+2	$8s^2 5g^{16} 8p^2$			
		$8s^2 5g^{17} 8p^1$		+0.2921	
	+4	$8s^2 6f^2 5g^{14}$			
	+6	$6f^1 5g^{15}$	2.428		r
		$8s^2 5g^{13}$		+0.6637	
	+7	$5g^{14}$			

3.3 The $8p^*$ shell

Mann and Waber^{26,27} found in their single-configuration jj -coupled DF calculations that, in the neutral atoms, one $8p^*$ electron appeared at E121-E125, and two at E126-. In the DS calculations of Fricke et al.¹⁹ the limits were E121-E126 and E127-, respectively.

For our electron book-keeping, we put the $8p^*$ shell at E139 and E140. As seen in Table 2 for the previous element, E138^{5+, 6+}, the available electrons will be placed in a full, $8s^2$

Period 1 Periodic Table 1-172 18 Orbitals

1	1 H	2											13	14	15	16	17	2 He	1s
2	3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne	2s2p
3	11 Na	12 Mg	3	4	5	6	7	8	9	10	11	12	13 Al	14 Si	15 P	16 S	17 Cl	18 Ar	3s3p
4	19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr	4s3d4p
5	37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe	5s4d5p
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	6s5d6p
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	114	115	116	117	118	7s6d7p
8	119	120	121-	156	157	158	159	160	161	162	163	164	139	140	169	170	171	172	8s7d8p
9	165	166											167	168				9s9p	

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	4f
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	5f
8	141	142	143	144	145	146	147	148	149	150	151	152	153	154	155	6f

8	121	122	123	124	125	126	127	128	129	130	131	132	133	134	135	136	137	138	5g
---	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	----

Fig. 3 The new, compact Periodic Table for elements 1-172. The numbers 1 - 18 are the Groups. For Periods 8 and 9, the Groups 13-14 are interpreted as p* (p_{1/2}) states and the Groups 15-18 as p (p_{3/2}) states. Please note that, in this most compact version and respecting the 'Orbitals' assignment in the right-hand marginal, the Z values do not increase systematically. An alternative were to break present Period 8 into the pieces 8a (119-120), 8b (139-140) and 8c (156-164, 169-172).

Table 3 Calculated electron configurations for nuclear charge Z and ionicity q for $Z > 140$. The quantity I is the energy of the next ionization

Z	q	El. conf.	$I/a.u.$	Exc. en.	
143	+6	$8s^1 5g^{18}$	2.652		
		$6f^1 5g^{18}$			
144	+7	$5g^{18}$	2.139		
	+5	$8s^2 6f^1 5g^{18}$			
	+6	$8s^2 5g^{18}$			
	+7	$8s^1 5g^{18}$			
	+8	$6f^1 5g^{18}$			+0.1269
		$5g^{18}$			
		$6f^1 5g^{17}$			+0.4306
		$8s^1 5g^{17}$			+0.4908
145	+6	$7d^1 5g^{17}$	2.783		
		$6f^1 5g^{17}$			+1.5227
	+7	$5g^{18} 8s^2 6f^1$	3.303		
		$5g^{18} 8s^1 6f^2$			+0.1737
	+8	$5g^{18} 8s^2$	3.755		
		$5g^{18} 8s^1 6f^1$			+0.0443
		$5g^{18} 6f^2$			+0.1755
	146	+9	$5g^{18} 6f^1$	4.494	
$5g^{18} 8s^1$			+0.0025		
+8		$5g^{18}$	3.836		
		$5g^{18} 8s^1 6f^1$			+0.0031
		$5g^{18} 6f^2$			+0.0887
147	+10	$5g^{18} 8s^2$	5.272		
		$5g^{18} 6f^1$			+0.1388
		$5g^{18} 8s^1$			
148	+11	$5g^{18}$	6.088		
		$5g^{18} 6f^1$			+0.2800
149	+12	$5g^{18} 8s^1$	6.940		

shell, the rest going to the 5g shell, and none yet to the 8p shell. This supports the present placement.

3.4 The 6f series

We here have a choice of keeping the $8s^2$ shell, or ionizing it away. If we keep it, we can place the 15 following elements E141-E155 below the actinides Ac-Lr. (Note that in the upper part of the PT, there is a slot at Group 3, and Ac, $7s^2 6d^1$, is usually included on the actinide row, giving fifteen items. In contrast to the actinides, which lose their 7s electrons in compounds, the present series, in their lower oxidation states, keep their $8s^2$ but formally lose the $(8p^*)^2$ electrons.

Taking as example the system E144⁺⁵ (see Table 3), it has an $8s^2 6f^1 5g^{18}$ configuration, and belongs in this sense to a 6f series. As its analog U⁵⁺ ($5f^1$), E144 in its lower oxidation state hence does belong to Group 6 on the 6f row of Period 8.

More generally, for the lower oxidation state of the 6f series, we expect an E1 18 core + a $5g^{18} 8s^2$ semicore + the remaining electrons, going to the $6f^k$ shell with

$$k = Z - 138 - i, \quad (3)$$

where i is the ionic charge. For the heavier 6f elements, see Table 4. As another example, the trivalent E155 will correspond to a $6f^{14}$ closed-shell configuration, like its analogs Lu and Lr in the suggested PT, Figure 3. Note that the 8p shell still remains above 6f in our EAL total-energy calculations. The $8p^* = 8p_{1/2}$ eigenvalue is comparable with the 6f ones at E155³⁺.

For the 6f series we also have the higher oxidation state, such as E144⁸⁺, where the 8s shell is ionized away. In fact, as the last electron above a $5g^{18}$ core, the 6f replaces the 8s starting from E145⁸⁺. The E146⁸⁺ has one of each, an $8s^1 6f^1$ configuration in the EAL model. This underlines the similar binding energies of the 8s and 6f electrons in this neighbourhood.

This situation may create for the 6f elements a large range of high oxidation states, as discussed in Chapter 5. This is also a bit analogous with the Groups 13-15 of Period 6, with the choice between Tl(I, III), Pb(II,IV) or Bi(III,V).

As seen from Table 4, at E153³⁺ the 8s shell is already clearly under the 6f. Similarly, in the pentavalent state, E155⁵⁺, the 8s electrons are kept but the 6f shell is ionized to $6f^{12}$.

For the higher oxidation state, the number of 6f electrons is

$$k = Z - 136 - i, \quad (4)$$

3.5 The 7d series

After the 6f series, we assign the nine elements E156-E164 formally to a 7d series in Groups 4-12.

Table 3 suggest 8p to lie slightly below 7d for E156³⁺. The $8p^*$ eigenvalue of -1.91 au is clearly below the SO-averaged 7d one of -1.14 au. Note that trivalent Ti, Zr and Hf are d^1 while E156³⁺ is p^1 but has a low-lying d^1 state.

As seen from Table 4, E156⁴⁺ is $8s^2 6f^{14}$. If ionized further to 5+ or 6+, the electrons are taken from the 6f, not from the 8s.

At the end of the series, the chemical properties of eka-copernicium, E164, were discussed by Penneman et al.⁵⁰. It was mainly predicted to be divalent, but oxidation states +IV and +VI were also expected. The calculated I_i for $i = 2 - 4$ in Table 3 lie above the limiting line in Figure 6, suggesting at most borderline chemical stability. Notice that, unlike Zn-Hg, but like Cn⁵¹, the ions of E164 keep both 8s electrons but remove 7d ones, which lie clearly higher. The $8s^2 7d^{10}$

ground-state configuration of E164 is analogous to all of Zn-Cn, which motivates keeping E164 in Group 12 of Period 8. This also fixes the positions of the preceding 7d elements.

3.6 The last main-group elements

The $9s^1$ and $9s^2$ elements E165 and E166 are now in Groups 1 and 2, respectively. Unlike the ns elements of Periods 3-8, which have an underlying np^6 core, the E165 and E166, however, have an underlying $7d^{10}$ core. In that sense, they would have a chance of rather being analogs to Au and Hg, or to Rg and Cn. and being members of Groups 11-12 of the Period 9, next to E167.

As seen from Table 3, the dication $E166^{2+}$ strongly prefers a $7d^{10}9s^0$ configuration to the alternatives $7d^99s^1$ or $7d^89s^2$. We recall here that Rg (E111) prefers a $6d^98s^2$ ground state⁵². Due to this orbital order $7d < 9s$, we therefore let E165 and E166 stay in Groups 1 and 2, as done by Fricke et al.¹⁹.

For the elements E167-E172 we likewise follow them in taking the energetic order as $9s < 9p_{1/2} < 8p_{3/2}$. Note that the SO splittings are so large that they are making two SO-split suborbitals with different n nearly degenerate.

4 Orbital radii

4.1 The nodeless 5g orbital

It is well-known that the first orbital with every l (1s, 2p, 3d, 4f, 5g, ...) is much more compact than the following orbitals with the same l . This was noticed for 3d and 4f orbitals by Jørgensen⁵³, who related it to the number of radial nodes (actually 'maxima', see his p. 46). Similar later arguments exist for the shells $2p$ ^{54,55} and $1s$ ⁵⁶. Also Slater⁵⁷ comments that the r_{\max} of the 3d shells of Sc-Ni, given earlier by himself⁵⁸, are 'much smaller than those for the 4s, even though the energies are about the same'. He mentions their 'different shapes'. Qualitatively one could say that the higher levels with the same l feel a *primogenic repulsion*⁵⁹ from the first, nodeless orbital. For a recent review on this problem, see Kaupp⁶⁰.

How compact is the 5g shell, compared with its counterparts? We show in Table 5 typical radii, $\langle r \rangle$, for the four series. The 5g shell is compact, but rather comparable with the other three series.

Estimates for the ionic radii of E104-E120 and E156-E172 were provided by Fricke and Waber⁶¹ as the r_{\max} of the outermost occupied orbital. The neutral atom r_{\max} of Waber et al.²⁴ for the 6f and 5g shells from E124 to E132 are comparable with the present values for their ions in Figure 4.

Because of the small size of the 5g shell, the 5g elements may rather chemically form a group of *superlanthanides*, in the sense of systematic magnetic behaviour, and non-participation of the 'label orbital' 5g in the formation of bonds.

The difference is that the lanthanides use 6s and 5d in their covalent bonds, but the 5g series has the panoply of 8s, $8p^*$, 7d and 6f for the purpose. For factors determining the ionic radii, see the subsection on $7p_{3/2}$ orbitals.

4.2 Magic numbers

The Lewis octets, corresponding to a formally filled ns^2np^6 electron configuration, are well-known. Likewise, the 18-electron rule with a formal $ns^2np^6(n-1)d^{10}$ -like configuration at the central atom is well-known; for its history and actual interpretation, see ref.⁶². The next step is a 32-electron closed-shell structure around a central atom. Recently, both the predicted $Pu@Pb_{12}$ ⁶³ or $Pu@Sn_{12}$ ⁶⁴ and the experimentally observed $U@C_{28}$ ⁶⁵ isoelectronic series were found to form good examples on such 32-electron systems.

To obtain the next, 50-electron magic number, the first chance would be the 6g shell which, however, remains outside the elemental range, studied here.

4.3 The $7p_{3/2}$ semicore orbital

In the PT, the 5p orbital is filled at Xe and becomes the core orbital of the lanthanides. Similarly, the 6p orbital is filled at Rn and becomes the semicore orbital of the actinides. Although so far not formally oxidized, it can strongly hybridize with the valence orbitals in systems like uranyl or UF_6 (for some references, see⁶⁶). We now notice that the $7p_{3/2}$ orbital, filled at E118, remains the largest core orbital up to about E164. It is only slightly more compact than the 8s one, when this becomes permanently occupied around E153. The r_{\max} values are shown in Figure 4.

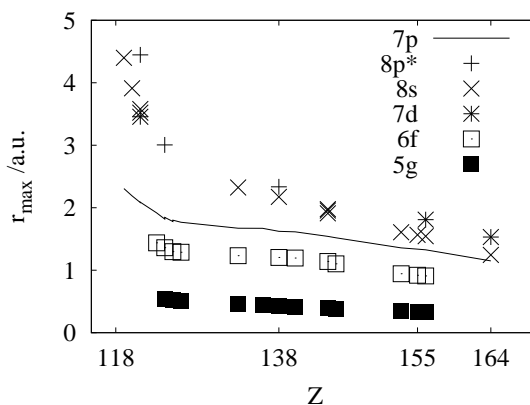


Fig. 4 The distances for maximum electron density for the orbitals 7p, 8s, $8p^*$, 7d, 6f and 5g for the systems indicated by an 'r' in Tables 2 and 3. Note that 7p (given by the line) remains the outermost core orbital until about E153.

5 Ionization potentials and oxidation states

Concerning the possible SHE oxidation states, Jørgensen⁶⁷ guessed for E126 an oxidation state of +IV ($5g^4$), while Fricke et al.¹⁹ thought its normal oxidation state could be as high as +8. Along the series, they expected a reduction to +6 at E132, and to +3 or +4 around E144.

As well-known in the chemical literature (e.g.^{68,69}), for electrons removed from the same atomic shell, the ionization potentials I_n systematically increase. Pyper and Grant^{70,71} rationalized this observation considering the atomic integrals involved.

How far along the atomic I_n sequence can we go in chemical compounds, assuming that the sum of the ionization energies is paid back by combined interionic Coulomb attractions and covalent bonding? Moreover it should be noticed that e.g. the Mulliken charges of the central atom can be roughly half of the formal oxidation state. An early example on this rule of thumb were the XeF_n ; $n=2-6$, (see ref.⁶⁶, Fig. 4).

Experimentally, oxidation states up to +VIII are now known in oxides and fluorides⁷². Himmel et al.⁷³, suggest gas-phase IrO_4^+ as a possible chemical system with oxidation state +IX. Parenthetically, the octahedral UO_6 has been predicted to exist as a local high-energy minimum^{74,75}. It is not really a U(XII) compound, in the sense of oxidizing the 6p semicore levels, and has, moreover, lower-lying peroxido and superoxido isomers.

Can we relate the ionization energies, I_i of the free ions to the maximum oxidation states in compounds? Certain I_i values are shown in Table 6 and a correlation between the two numbers is shown in Figure 5. This, rather Gordian, empirical attempt may give some idea of the possible oxidation states, if the I_i is known.

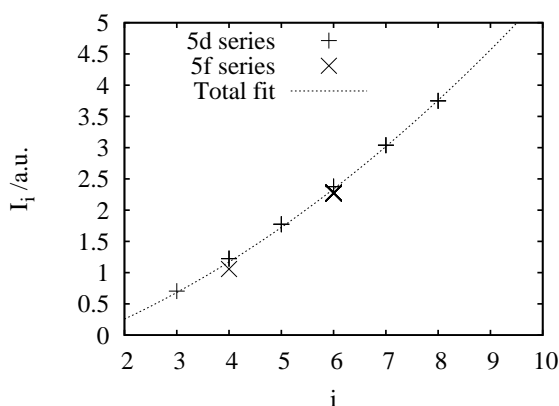


Fig. 5 The correlation between the free-ion last ionization energies, I_i , and the maximum known oxidation state, i for certain 5d and 5f elements. The data are taken from Table 6.

We then compare some calculated ionization energies for the present SHE in Figure 6. For the nominal 5g series, the last valence electron is 8s, 6f and 5g for E121-122, E123-124 and E125-126, respectively. The values reach the line of Figure 5 at I_8 . A further ionization, leading to a $7p^5$ configuration, would have a much higher ionization energy, e.g. an I_7 of 3.184 au for E124.

The curve for the higher oxidation state of the 6f series lies below the experimentally known cases, making them also plausible, possibly to some very high i values, such as $i = 12$ for the hypothetical (E148) O_6 . A further study would require molecular calculations.

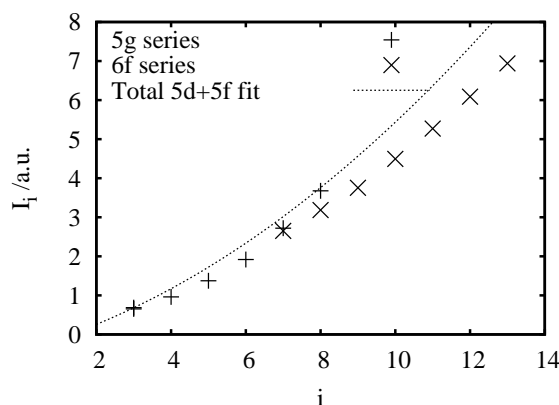


Fig. 6 A comparison of some present calculated ionization energies with the fit to experimentally known maximum ones in Figure 5. The '6f' series corresponds to the higher oxidation state.

6 Multi-shell transition metals?

Taking an example, it is known that the Gd atom ground state is $6s^2 5d^1 4f^7$, with open 5d and 4f shells. For neutral or nearly neutral SHE this also is a common occurrence. Could this occur in compounds, or the present highly-charged ions?

Table 2 has $E138^{+6}$ with a low-lying $6f^1 5g^{13}$ configuration. $E140^{+6}$ has a $6f^1 5g^{15}$ ground state. Thus some 6f-5g overlap may occur in this neighbourhood.

7 Possible new molecules

Some characteristic molecules for the presently studied 5g, 6f and 7d elements are given in Table 7. Their theoretical verification must be left to future quantum chemical studies. The $5g^0$ cases in the beginning are analogs of lanthanides in the sense of having a compact, inner shell, being filled.

Table 6 Successive ionization potentials (in au), I_n (in au) for certain elements. 'Chemically unknown' ionizations are given in italics.

Atom	I_1	I_2	I_3	I_4	I_5	I_6	I_7	I_8	Source
La	0.20495	0.4064	0.7047	<i>1.836</i>					76
Hf	0.2508	0.55	0.856	1.225					77
Ta	0.290	0.569	0.872	1.36	1.774				78
W	0.2890	0.589	0.950	1.396	1.884	2.377			79
Re							3.0395		80
Os								3.7493	80
Th	0.2318	0.437	0.735	1.058					77
U	0.233	0.411	0.707	1.171	1.711	2.274	3.268		81

8 Conclusions

Based on the present ionic calculations, we have found a way to split the very long row E121-E164 of Fricke et al.¹⁹ to the suggested 5g, 6f and 7d segments, used in the present Figure 3. Especially the 6f series may possess some very high oxidation states.

While most experimental verifications may take a while, relativistic quantum chemistry could be used to show that e.g. (E125)F₆ is indeed 5g¹, as calculated by Makhyoun⁴³. It is similarly expected that (E143)F₆ and/or (E145)F₆ would be 6f¹ systems, and so on.

9 Acknowledgments

The author belongs to the Finnish Centre of Excellence of Computational Molecular Science (CMS). Dr. Jean-Paul Desclaux provided the version of the Dirac-Fock program used⁴⁶. Dr. Michiko Atsumi showed, how to use Excel for making the Figures 1 and 3. Dr. Valeria Pershina suggested and provided Figure 2.

References

- M. Kaji, *Found. Chem.*, 2003, **5**, 189–214.
- M. D. Gordin, *A Well-Ordered Thing: Dmitrii Mendeleev and the Shadow of the Periodic Table*, Basic Books, New York, 2004.
- E. R. Scerri, *The Periodic Table. Its Story and Its Significance*, Oxford Univ. Press, Oxford, 2007.
- V. N. Ostrovsky, *Ann. N. Y. Acad. Sci.*, 2003, **988**, 182–192.
- M. Kibler, *Found. Chem.*, 2007, **9**, 221–234.
- S.-G. Wang and W. H. E. Schwarz, *Angew. Chem. Int. Ed.*, 2009, **48**, 3404–3415.
- W. H. E. Schwarz and S.-G. Wang, *Int. J. Quantum Chem.*, 2010, **110**, 1455–1465.
- W. H. E. Schwarz and R. L. Rich, *J. Chem. Ed.*, 2010, **87**, 435–443.
- Anon., *old.iupac.org/reports/periodic-table*, Downloaded 20 August 2010.
- G. T. Seaborg, *J. Chem. Soc. Dalton Trans.*, 1996, 3899–3907.
- Yu. Ts. Oganessian, F. Sh. Abdullin, P. D. Bailey, D. E. Benker, M. E. Bennett, S. N. Dmitriev, J. G. Ezold, J. H. Hamilton, R. A. Henderson, M. G. Itkis, Yu. V. Lobanov, A. N. Mezentsev, K. J. Moody, S. L. Nelson, A. N. Polyakov, C. E. Porter, A. V. Ramayya, F. D. Riley, J. B.

- Roberto, M. A. Ryabini, K. P. Rykaczewski, R. N. Sagaidak, D. A. Shaughnessy, I. V. Shirokovsky, M. A. Stoyer, V. G. Subbotin, R. Sudo, A. M. Sukhov, Yu. S. Tsyganov, V. K. Utyonkov, A. A. Voinov, G. K. Vostokin and P. A. Wilk, *Phys. Rev. Lett.*, 2010, **104**, 142502.
- M. Schädel, *J. Nucl. Radiochem. Sci.*, 2002, **3**, 113–120.
- M. Schädel, *Angew. Chem. Int. Ed.*, 2006, **45**, 368–401.
- D. C. Hoffman, In *The Robert A. Welch Foundation Conference on Chemical Research. XXXIV. Fifty Years With Transuranium Elements*, Houston, Texas, 1990, 255–276.
- V. Pershina, In *Relativistic Electronic Structure Theory. Part 2. Applications*, Ed. P. Schwerdtfeger, Amsterdam, 2004, pp. 1–80.
- V. Pershina, *Radiochim. Acta*, 2005, **93**, 125–131.
- P. Pyykkö and M. Atsumi, *Chem. Eur. J.*, 2009, **15**, 186–197.
- P. Pyykkö, S. Riedel and M. Patzschke, *Chem. Eur. J.*, 2005, **11**, 3511–3520.
- B. Fricke, W. Greiner and J. T. Waber, *Theor. Chim. Acta*, 1971, **21**, 235–260.
- B. Fricke, *Struct. Bonding*, 1975, **21**, 89–144.
- B. Fricke and J. T. Waber, *Actinides Rev.*, 1971, **1**, 433–485.
- B. Fricke and G. Soff, *At. Data Nucl. Data Tables*, 1977, **19**, 83–95.
- J. T. Waber, In "Proc. 13th R A Welch Foundation Conf. on Chem. Res., The Transuranium Elements", Houston, TX, 1969, 353–443.
- J. T. Waber, D. T. Cromer and D. Liberman, *J. Chem. Phys.*, 1969, **51**, 664–668.
- C. C. Lu, T. A. Carlson, F. B. Malik, T. C. Tucker and C. W. Nestor Jr., *Atomic Data*, 1971, **3**, 1–131.
- J. B. Mann, *J. Chem. Phys.*, 1969, **51**, 841–842.
- J. B. Mann and J. T. Waber, *J. Chem. Phys.*, 1970, **53**, 2397–2406.
- I. Pomeranchuk and J. Smorodinsky, *J. Phys. (USSR)*, 1945, **9**, 97–99.
- F. G. Werner and J. A. Wheeler, *Phys. Rev.*, 1958, **109**, 126–144.
- B. Müller, J. Rafelski and W. Greiner, *Nuovo Cim. A*, 1973, **18**, 551–573.
- Ya. B. Zel'dovich and V. S. Popov, *Usp. Fiz. Nauk*, 1971, **105**, 403–440; *Sov. Phys. Uspekhi*, 1972, **14**, 673–824.
- V. S. Popov, *Phys. At. Nuclei*, 2001, **64**, 367–392; *Yad. Fiz.*, 2001, **64**, 421–446.
- P. Pyykkö, M. Tokman and L. N. Labzowsky, *Phys. Rev. A*, 1998, **57**, R689–R692.
- L. Labzowsky, I. Goidenko, M. Tokman and P. Pyykkö, *Phys. Rev. A*, 1999, **59**, 2707–2711.
- P. Pyykkö and L.-B. Zhao, *J. Phys. B*, 2003, **36**, 1469–1478.
- P. Indelicato, J. P. Santos, S. Boucard and J.-P. Desclaux, *Eur. Phys. J. D*, 2007, **45**, 155–170.
- J. P. Desclaux, *At. Data Nucl. Data Tables*, 1973, **12**, 311–406.
- K. Umemoto and S. Saito, *J. Phys. Soc. Japan*, 1996, **65**, 3175–3179.
- E. Eliav, A. Landau, Y. Ishikawa and U. Kaldor, *J. Phys. B*, 2002, **35**, 1693–1700.
- V. I. Nefedov, M. B. Trzhaskovskaya and V. G. Yarzhevskii, *Doklady*

Phys. Chem., 2006, **408**, 149–151.

- 41 E. Eliav, U. Kaldor, Y. Ishikawa and P. Pyykkö, *Phys. Rev. Lett.*, 1996, **77**, 5350–5352.
- 42 I. Goidenko, L. Labzowsky, E. Eliav, U. Kaldor and P. Pyykkö, *Phys. Rev. A*, 2003, **67**, 022102.
- 43 M. A. Makhyoun, *J. Chim. Phys.*, 1988, **85**, 917–924.
- 44 G. L. Malli, *J. Chem. Phys.*, 2006, **124**, 071102.
- 45 C. Thierfelder, P. Schwerdtfeger, A. Koers, A. Borschevsky and B. Fricke, *Phys. Rev. A*, 2009, **80**, 022501.
- 46 J. P. Desclaux and P. Indelicato, *The relativistic atomic program MCD-FGME V 2005.10*, Published at <http://dirac.spectro.jussieu.fr/mcdf/> on August 17, 2005, 2005.
- 47 E. Eliav, S. Shmulyian, U. Kaldor and Y. Ishikawa, *Phys. Rev. A*, 1998, **58**, 3954–3958.
- 48 T. H. Dinh, V. A. Dzuba, V. V. Flambaum and J. S. M. Ginges, *Phys. Rev. A*, 2008, **78**, 022507.
- 49 T. H. Dinh, V. A. Dzuba, V. V. Flambaum and J. S. M. Ginges, *Phys. Rev. A*, 2008, **78**, 054501.
- 50 R. A. Penneman, J. B. Mann and C. K. Jørgensen, *Chem. Phys. Lett.*, 1971, **8**, 321–326.
- 51 E. Eliav, U. Kaldor and Y. Ishikawa, *Phys. Rev. A*, 1995, **52**, 2765–2769.
- 52 E. Eliav, U. Kaldor, P. Schwerdtfeger, B. A. Hess and Y. Ishikawa, *Phys. Rev. Lett.*, 1994, **73**, 3203–3206.
- 53 C. K. Jørgensen, *Energy Levels of Complexes and Gaseous Ions*, Thesis, Gjellerups Forlag, Copenhagen, 1957.
- 54 P. Pyykkö, *J. Chem. Research (S)*, 1979, **1979**, 380–381.
- 55 W. Kutzelnigg, *Angew. Chem. Int. Ed. Engl.*, 1984, **23**, 272–295.
- 56 P. Pyykkö, *Int. J. Quantum Chem.*, 2001, **85**, 18–21.
- 57 J. C. Slater, *Quantum Theory of Atomic Structure, Vol. 1*, McGraw-Hill, New York, 1st edn, 1960.
- 58 J. C. Slater, *Introduction to Chemical Physics*, McGraw-Hill, New York, 1st edn, 1939.
- 59 P. Pyykkö, *Phys. Scr. (Sweden)*, 1979, **20**, 647–651.
- 60 M. Kaupp, *J. Comp. Chem.*, 2007, **28**, 320–325.
- 61 B. Fricke and J. T. Waber, *J. Chem. Phys.*, 1972, **56**, 3246.
- 62 P. Pyykkö, *J. Organomet. Chem.*, 2006, **691**, 4336–4340.
- 63 J.-P. Dognon, C. Clavaguéra and P. Pyykkö, *Angew. Chem. Int. Ed.*, 2007, **46**, 1427–1430.
- 64 J.-P. Dognon, C. Clavaguéra and P. Pyykkö, *Compt. Rend. Chimie*, 2010, **13**, 884–888.
- 65 J.-P. Dognon, C. Clavaguéra and P. Pyykkö, *J. Am. Chem. Soc.*, 2009, **131**, 238–243.
- 66 S. Larsson and P. Pyykkö, *Chem. Phys.*, 1986, **101**, 355–369.
- 67 C. K. Jørgensen, *Chem. Phys. Lett.*, 1968, **2**, 549–550.
- 68 C. K. Jørgensen, *Angew. Chem. Int. Ed.*, 1973, **12**, 12–19.
- 69 C. S. G. Phillips and R. J. P. Williams, *Inorganic Chemistry. I*, Clarendon Press, Oxford, 1965. See pp. 47–52.
- 70 N. C. Pyper and I. P. Grant, *Proc. Roy. Soc. (London) A*, 1978, **360**, 525–543.
- 71 N. C. Pyper and I. P. Grant, *J. Chem. Soc. Faraday 2*, 1978, **74**, 1885–1900.
- 72 S. Riedel and M. Kaupp, *Coord. Chem. Rev.*, 2009, **253**, 606–624.
- 73 D. Himmel, C. Knapp, M. Patzschke and S. Riedel, *ChemPhysChem*, 2010, **11**, 865–869.
- 74 H. Xiao, H.-S. Hu, W. H. E. Schwarz and J. Li, *J. Phys. Chem. A*, 2010, **114**, 8837–8844.
- 75 P. Pyykkö, N. Runeberg, M. Straka and K. G. Dyall, *Chem. Phys. Lett.*, 2000, **328**, 415–419.
- 76 W. C. Martin, L. Hagan, J. Reader and J. Sugar, *J. Phys. Chem. Ref. Data*, 1974, **3**, 771–779.
- 77 D. R. Lide (Ed.), *CRC Handbook of Chemistry and Physics, 90th Ed.*

2009–2010, CRC, Boca Raton, FL, 2010.

- 78 B. Fricke, E. Johnson and G. M. Rivera, *Radiochim. Acta*, 1993, **62**, 17–25.
- 79 E. Johnson, V. Pershina and B. Fricke, *J. Phys. Chem. A*, 1999, **103**, 8458–8462.
- 80 J. Sugar and V. Kaufman, *J. Opt. Soc. Am.*, 1979, **69**, 141–143.
- 81 C. R. A. Catlow, *J. Chem. Soc., Faraday 2*, 1978, **74**, 1901–1908.
- 82 C. Clavaguéra, J.-P. Dognon and P. Pyykkö, *Chem. Phys. Lett.*, 2006, **429**, 8–12.
- 83 M. Straka, K. G. Dyall and P. Pyykkö, *Theor. Chem. Acc.*, 2001, **106**, 393–403.
- 84 X.-F. Wang, L. Andrews, S. Riedel and M. Kaupp, *Angew. Chem. Int. Ed.*, 2007, **46**, 8371–8375.

Periodic Table I-172

1	2											13	14	15	16	17	18	Orbitals		
1	H																1s			
2	3	4										5	6	7	8	9	10	2s2p		
	Li	Be										B	C	N	O	F	Ne			
3	11	12	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	3s3p	
	Na	Mg											Al	Si	P	S	Cl	Ar		
4	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	4s3d4p	
	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr		
5	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	5s4d5p	
	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe		
6	55	56	57	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86	6s5d6p	
	Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn		
7	87	88	89	104	105	106	107	108	109	110	111	112	113	114	115	116	117	118	7s6d7p	
	Fr	Ra	Ac	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Uu	Uu	Uu	Uu	Uu	Uu		
8	119	120	121	122	123	124	125	126	127	128	129	130	131	132	133	134	135	136	8s7d8p	
9	165	166											167	168					9s9p	
6	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71				4f	
	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu					
7	89	90	91	92	93	94	95	96	97	98	99	100	101	102	103				5f	
	Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr					
8	141	142	143	144	145	146	147	148	149	150	151	152	153	154	155				6f	
8	121	122	123	124	125	126	127	128	129	130	131	132	133	134	135	136	137	138	5g	

Fig. 7 Graphical Abstract: The last valence electrons, left on an ion, are used to assign the superheavy elements E121–E164 to individual (nlj) slots. A compact Periodic Table up to E172 is obtained.

Table 4 Calculated electron configurations for nuclear charge Z and ionicity q for $Z > 153$. The quantity I is the energy of the next ionization

Z	q	El. conf.	$I/a.u.$	Exc. en.
153	+1	$8s^2 6f^{14}$	0.380	
	+2	$8s^2 6f^{13}$	0.872	
	+3	$8s^2 6f^{12}$	1.415	
		$8s^1 6f^{13}$		+0.5810
		$6f^{14}$		+1.2253
	+4	$8s^2 6f^{11}$	1.999	
	+5	$8s^2 6f^{10}$	2.619	
+6	$8s^2 6f^9$	3.270	r	
155	+3	$8s^2 6f^{14}$	1.484	
	+4	$8s^2 6f^{13}$	2.084	
	+5	$8s^2 6f^{12}$	2.720	r
		$8s^1 6f^{13}$		+0.4201
		$6f^{14}$		+0.9189
+6	$8s^2 6f^{11}$			
156	+3	$8p^1$	1.177	
		$7d^1$		+0.0538
	+4	$8s^2$	2.126	
	+5	$8s^2 6f^{13}$	2.770	r
		$8s^1 6f^{14}$		+0.4434
+6	$8s^2 6f^{12}$			
158	+3	$7d^1 8p^2$		
164	+1	$7d^9 8s^2 8p^2$	0.888	
			0.600 ^a	
	+2	$7d^8 8s^2 8p^2$	1.300	
	+3	$7d^7 8s^2 8p^2$	1.741	r
	+4	$7d^6 8s^2 8p^2$		
166	+2	$7d^{10} 8p^2$		
		$9s^1 7d^9 8p^2$		+0.5826
		$9s^2 7d^8 8p^2$		+1.2594
168	+2	$8p^4$		
		$9s^1 8p^3$		+1.0742
		$9s^2 8p^2$		+2.2027

^a Single-configuration jj -coupled DF, ref. ⁵⁰.

Table 7 Some possible molecules, containing the 5g, 6f and 7d elements E121-E164. X is a halogen, O oxygen.

Class	Molecules	Analogs	
$8s^0 5g^0$	(E121)X ₃	LaX ₃ ⁸²	
	(E122)X ₄		
	(E123)X ₅		
	(E124)X _{6,...}		
	(E126)O ₄		
	(E125)X ₆ ^a		
$8s^0 5g^1$	$8s^2(8p^*)^0 6f^0 5g^{18}$	ThF ₄	
	(E142)X ₄	UF ₆	
	(E144)X ₆	UO ₂ ²⁺	
	(E144)O ₂ ⁺	PuF ₈ ⁸³	
	(E144)F ₈	PuO ₄ ⁸³	
	(E144)O ₄	UO ₆ ^{74,75}	
$8s^0(8p^*)^0 6f^0 5g^{18}$	(E148)O ₆		
	(E142)X ₆	WF ₆ , SgF ₆	
	$8s^2(8p^*)^0 7d^0 6f^{14} 5g^{18}$	(E158)X ₆	OsO ₄ , HsO ₄
	(E160)O ₄		
	$8s^0(8p^*)^0 7d^0 6f^{14} 5g^{18}$	(E158)X ₈	
	(E158)O ₄		
$8s^2(8p^*)^0 7d^{10} 6f^{14} 5g^{18}$	(E164)X ₂	HgX ₂	
	$8s^2(8p^*)^0 7d^8 6f^{14} 5g^{18}$	(E164)X ₄	HgF ₄ ⁸⁴
	(E164)X ₄		

^a Done in ref. ⁴³.

Table 5 The decrease of the average radius $\langle r \rangle$ for the nodeless atomic orbitals from DF calculations. Desclaux's tables for neutral atoms³⁷ are used for the 1s, 2p, 3d and 4f series. Present data for the 5g examples.

Series	Beginning		End	
	Atom	$\langle r \rangle$	Atom	$\langle r \rangle$
1s	H	1.5	He	0.927
2p	B	2.205	Ne	0.964
3d	Sc	1.692	Cu	0.998
4f	Ce	1.041	Lu	0.702
5g	E124 ⁵⁺	0.756	E140 ⁶⁺	0.593