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Is the Periodic Table all right (“PT OK”)?

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Abstract. The history of the Periodic Table and its predecessors spans almost 200 years. The present IUPAC PT for $Z = 1-118$ is still adequate. The remarkable measurement for the Lr atom does not change the chemistry. The extensions up to $Z = 172$ are discussed and compared. New data for ions are presented. The “Madelung rule” is found to be surprisingly good even in that range.

1. Introduction

The standard Periodic Table (PT) for the first 118 elements is shown in Fig. 1. Note that we have followed the IUPAC in putting the 15 elements La-Lu in a lanthanide row, and the 15 elements Ac-Lr in an actinide row, corresponding to a hole in Group 3 for Periods 6 and 7, respectively. This is entirely logical if we count the f -elements from f^0 to f^{14} .

A fine point is that for instance Th is counted as an f -element, despite of having a $7s^26d^2$ atomic ground state. In molecules or solids it may have a certain amount of $5f$ character. In the same sense E118 (Og), [Li, Be, Mg, Zn], [Cs, Ca, Sr, Ba] and Th could be called *pre-s*, *pre-p*, *pre-d* and *pre-f* elements, respectively [2]. The example for E118 was the existence of the atomic anion [3], Og^- , using the preliminary proposed name of Oganesson, Og.

As discussed in the lecture by Sato, the atomic ground state of the Lr atom is $(7p_{1/2})^1$, see Ref. [4], not $6d^1$, like the $5d^1$ ground state for Lu. Note that their experimental first ionization potential was $4.96_{(0.07)}^{(0.08)}$ eV, compared with their own theoretical value of 4.963(15) eV. The $6d$ level is only calculated to lie only 0.18 eV higher. However, the three first ionization potentials in Fig. 2 and the nature of the covalent bonds to Lu and Lr in a number of molecules are very similar [5]. Therefore changes in the PT are not proposed.

A brief history of the PT is given below in Sect. 3.

2. How to continue the PT beyond $Z = 118$?

2.1 The long-row proposal of Fricke *et al.* [6]

In 1971 Fricke *et al.* [6] reported Dirac-Slater (DS) calculations on neutral atoms up to $Z = 172$. This method could be called a primitive density functional approach, using the so-called Slater exchange. The limit at 172 is imposed by the diving of the lowest, $1s$ state in the lower, positron-like continuum. The nuclei were simply assumed to be there and assigned realistic Fermi charge distributions.

They found considerable occupational overlap of the $8s$, $8p$, $7d$, $6f$, and $5g$ shells, and no big gaps between any of them. This motivated putting the elements 119–164 on one

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Periodic Table 1-118, April 2016

Period	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- 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- Ac	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	7s6d7p					
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					

Figure 1. The standard Periodic Table for the 118 first elements. Adapted from Pyykkö [1].

very long row, followed by a shorter row for elements 165–172. The new feature was the large spin-orbit splitting of the $8p$ and $9p$ shells and the large relativistic stabilization of the $9s$ shell.

2.2 The short-rows proposal of Pyykkö [1]

It would offer at least a typographical advantage to have shorter rows. Moreover, the effective charges of these heavy atoms in compounds can often be expected to be positive, possibly strongly positive. For simplicity, one can study the electronic behaviour of monoatomic cations. These calculations were carried out by the Extended Average Level Multiconfiguration Dirac-Fock (EAL MCDF) method using the code of Desclaux and Indelicato [7]. Again, a realistic nuclear model was assumed, assuming that the nuclei are there.

All available calculations (see [1]) predict for E119 and E120 an $8s^1$ and $8s^2$ electron configuration, respectively. In the extreme case, assume that there is only one valence electron and ask, what does it want to do? If one raises the nuclear charge, the single valence electron remains an $8s$ for $Z = 120$ – 122 but then prefers $6f$ for $Z = 123$ – 124 and finally turns to $5g$ for $Z \geq 125$, see Fig. 3. Similar results lead to a formal assignment of all the elements 121–138 to a $5g$ series, often in a *pre-5g* sense [1]. Recall the ‘actinide’ Th.

A second example motivating this assignment of a $5g$ row is the calculation of Indelicato *et al.* [8], who find an $8s^2(8p_{1/2})^25g^{18}$ closed-shell electron configuration for the isoelectronic series to the E140 atom of $Z = 143$ – 148 . Thirdly, neutral-atom calculations start to occupy the first $5g$ states around E125 [6, 9–11] or E126 [12].

We summarize the short-row 172-element PT in Fig. 4.

2.3 The Madelung mnemonic rule

It is almost disappointing that the simple $(n + l, n)$ “Madelung rule” still seems to hold. Shells are filled in the order of: 1) Increasing $N = n + l$ and, 2) For same N , largest n .

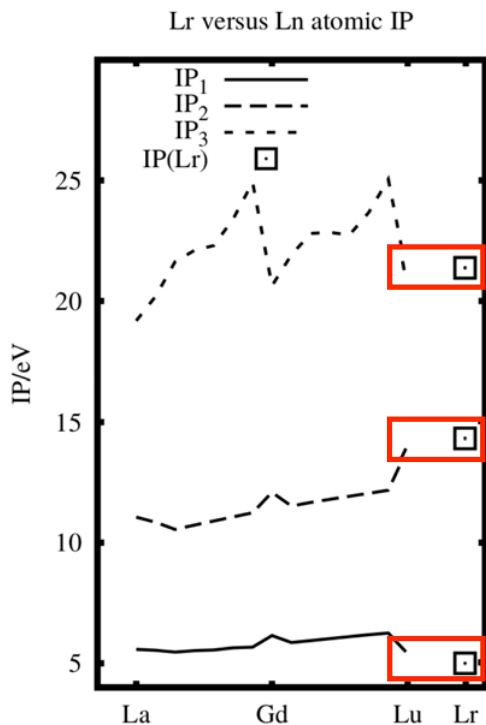


Figure 2. The ionization potentials IP_{1-3} of the lanthanides La-Lu and of Lr. Note the similarity of the values for Lu and Lr. From Ref. [5].

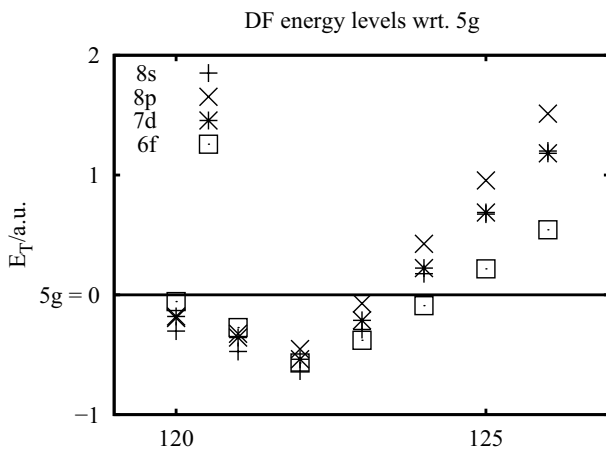


Figure 3. The lowest occupied states of a $[118e]+1e$ alkali-like atom for various nuclear charges. The 5g energy is defined as zero. Previously unpublished.

Periodic Table 1-172

Period 1	Periodic Table 1-172																		18 Orbitals	
1	1 H	2											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar	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- 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- Ac	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	7s6d7p	
8	119	120	121- 103	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
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Figure 4. The PT proposed by Pyykkö. Modified from [1] by adding the year-2016 preliminary name proposals, and by emphasizing the non-monotonous cases by colour.

The "Madelung rule" up to $Z = 172$

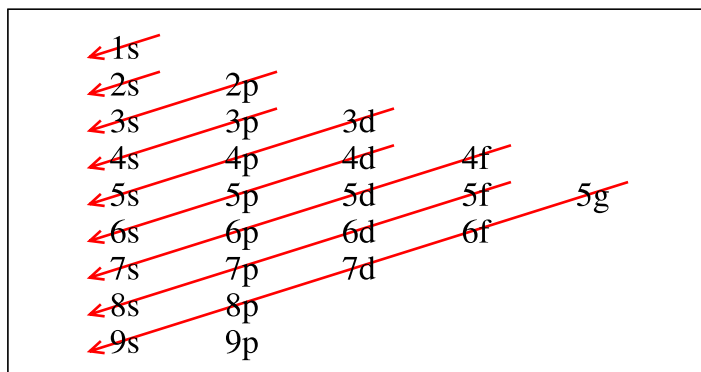


Figure 5. The "Madelung rule" applied in the present case. Previously unpublished.

The occupation order in the 172-element PT of Fig. 4 closely follows the "Madelung" occupation order in Fig. 5. For the 8th and 9th Period in Fig. 4 this amounts to

$$8s < 5g < 6f < 7d < 8p < 9s. \quad (1)$$

This is only broken up by the large spin-orbit splitting for the 8p and 9p shells, and the large relativistic stabilization of the 9s shell.

Actually the “Madelung” occupation order is also close to that obtained from the old quantum theory by Niels Bohr. In his Nobel lecture [13] he talks about the *number of quanta*, meaning in modern atomic theory the number of radial half-waves plus the number of angular nodes.

For more literature on the Madelung rule, see Ostrovsky [14].

3. History of the Periodic Table

For literature on the history of the PT we recommend the book of Scerri [15] and the paper of Wang and Schwarz [16]. The earliest work was based on atomic weights. The first fragments were the “triads” of Döbereiner: (Ca, Sr, Ba) in 1817 and (Li, Na, K), (S, Se, Te), (Cl, Br, I) in 1829. Gmelin in 1843 had a table of 55 elements, having oxygen in the correct group, and discussing chemical properties. The 1860 Karlsruhe conference (with a 150-year celebration in Karlsruhe in 2010) was instrumental in summarizing the data. Following the *vis tellurique* of de Chancourtois in 1862 and the *octaves* of Newlands in 1863 and 1865, Meyer (1864) had a table of 28 elements with gaps. Mendeleev in 1869 had a table explicitly predicting missing elements with atomic weights of 45, 68 and 70. These were discovered shortly afterwards and were named Sc, Ga and Ge, respectively. The group of noble gases was reported by Ramsay in 1900. Finally, Seaborg introduced the actinide row in 1945. So far the *6d* elements have been chemically boringly similar to their *5d* analogues, but this may change towards the end of the series [17].

4. Conclusion

The Periodic Table for the first 118 elements seems well settled, if one chooses 15-element lanthanide and actinide rows, corresponding to f^0 -to- f^{14} trivalent ions. Then one has to note that Th is counted as an actinide, although the neutral atom still has no *5f* electrons. In compounds Th may have some *5f* character.

Beyond the element 118 (preliminarily named Oganesson), the next two are expected to be *s*-elements, an alkali metal and an alkaline earth. For the subsequent elements we here consider at least two choices. In the present, “short rows” suggestion [1], the elements 121–138 are counted as *5g* elements. Then follow the $8p_{1/2}$ elements 139–140, the *6f* elements 141–155 and the *7d* elements 156–164. In the “long rows” suggestion of Fricke *et al.* [6] overlaps between these shell occupations are allowed. Fricke considered neutral atoms while the present author included ions.

Actually the Periodic Table is about chemistry, and one should consider compounds. Little information is yet available beyond element 118.

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