

Conference paper

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An essay on periodic tables

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Abstract: After a compact history of the PT, from Döbereiner's triads to the theoretical predictions up to element 172, a number of particular issues is discussed: Why may $Z=172$ be a limit for stable electron shells? What are the expected stability limits of the nuclear isotopes? When are formally empty atomic orbitals used in molecular electronic structures? What is 'Secondary Periodicity'? When do the elements (Ir, Pt, Au), at the end of a bond, simulate (N, O, I), respectively? Some new suggestions for alternative PTs are commented upon. As a local connection, Johan Gadolin's 1794 analysis of the Ytterby mineral is mentioned.

Keywords: analogies between elements; chemical bonding; lanthanides; Mendeleev 150; periodic tables; secondary periodicity; superheavy elements.

Historical introduction

A periodic table of elements (PT) arranges chemical elements as a function of their properties – how so? Any student might answer: by their nuclear charge, Z . Currently the elements with $Z=1-118$ have been found in nature or artificially produced. What did people use in the 19th century, before they knew about nuclei or nuclear charges? Atomic weights, m . Except for a few anomalies, arrangement by m gave the same running order towards heavier elements, as by Z .

History in a nutshell. The periodic behaviour of chemical elements slowly became apparent in fragments, perhaps beginning with Döbereiner's *triads*, such as (Ca, Sr, Ba) in 1817 or (Li, Na, K), (S, Se, Te) and (Cl, Br, I) in 1829. In each of these triads, the m of the second element is approximately equal to the average of the first and third.

In 1843, Gmelin had a table of 55 elements, with oxygen in the correct place. Following the spiralized 'telluric screw' (de Chancourtois 1862) and the Law of 'octaves' (Newlands 1863, 1865), Meyer constructed a square table of 28 elements (with gaps) in 1864. In 1869, Mendeleev wrote two articles (one in Russian and the other – a short summary – in German) explicitly predicting the existence of three missing elements with the atomic weights 45, 68 and 70. These were discovered in 1879, 1875 and 1886, and are now known as scandium (Sc; atomic weight 44.956), gallium (Ga; atomic weight 69.723) and germanium (Ge; atomic weight 72.640), respectively.

Mendeleev's articles (1869) also overlapped with the writing of his textbook *Fundamentals of Chemistry* (see Kaji [1]).

In 1900 Ramsay suggested that the new (nearly) noble gases should form a separate group, which is currently referred to as Group 18. Similarly, in 1945, Seaborg proposed that the newly discovered actinides

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Group	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	Orbital
1	1 H																	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											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-Ce	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-Lr	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- 124	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. 1: The present Periodic Table (yellow) and possible assignments of the future elements E119–E172 (white). Picture reproduced from Haba [2]. Table reproduced from Pyykkö [3, 4]. Note the p-orbital spin-orbit-induced anomalies at E139–140 and E167–168, and the 9s-orbital-induced location of E165–166.

should form their own row below the lanthanides. He purposely chose the elemental names europium, americium (Eu, Am), gadolinium, curium (Gd, Cm), and terbium, berkelium (Tb, Bk) to emphasize the (4f, 5f) analogy by selecting for these actinides names of a continent, a celebrated scientist, and a town.

Accelerator experiments have now completed the 6d series Rf–Cn and the 7p series Nh–Og, resulting in the currently accepted PT (highlighted in yellow in Fig. 1).

The theoretical predictions (shown in white in Fig. 1) by the present author [3, 4] support the idea of two 8s elements (E119 and 120), an overlapping ‘grey’ zone of additional shells (8p, 7d, and 6f) at E121–124, and then a systematic sequence of increasing 5g occupation numbers for the elements E125 onwards. Nominally, all of the elements E121–138 are assigned to a ‘5g’ series. As a parallel case, recall that we regard Th as an actinide, although the free thorium atom has no 5f orbital occupation. Accordingly, a name *pre-f* was recently introduced [5].

As a further data point supporting Fig. 1, Indelicato et al. [6a] find an $8s^2 8p^2 5g^{18}$ configuration for the cations E143³⁺ to E148⁸⁺. The atomic calculations on the superheavy elements (SHE) range from the Dirac-Slater (DS) ones by Fricke et al. [6b], and the Dirac-Fock (DF) ones by Desclaux [6c] to massive multiconfiguration DF (MCDF) approaches, such as [6a], and sophisticated many-body approaches [6d, 6e]. As an ultimate example, see [35] below. As to molecules, theoretical calculations on hypothetical octahedral hexafluorides, MF₆, support the onset of the expected 5g occupation from E125 to at least E129. Note that the metal atom, M, delivers six electrons to the six fluorides. The other valence electrons go to the 5g shell. These molecular relativistic density-functional calculations were reported by Dognon and Pyykkö [7]¹.

For more comprehensive treatises on the history of the PT, see Gordin [8], Kaji [1] or Scerri [9].

¹ The very compact size of the 5g shell would make these elements ‘superlanthanides’.

Technical details

Why must Z be ≤ 172 ?

The current border of the PT at $Z=118$ is set by the nuclear instability of the existing isotopes and by their small nucleosynthetic cross sections. For discussing chemical properties, even if the nuclei existed, there may also be limits, arising from the chemical reactivity of the vacuum in strong Coulomb fields, due to quantum electrodynamics, QED.

For any elements beyond E172, or so, the lowest or $1s$ shell would dive to the lower, positron-like continuum of the Dirac equation. It is not yet fully understood what would physically happen. Another way to study the question is to consider heavy-atom collisions [10]. For one, point-like nucleus this diving would already take place at $Z=137$. For the earlier literature on this question, see [3], p. 162.

Relativity vs. QED

It is well-known that the (Dirac) relativistic effects contract and stabilize the ns and np^* ($=np_{1/2}$) shells while the ensuing indirect relativistic effects expand and destabilize the d and f shells. As previously discussed [5], the QED effects, dominated by the vacuum fluctuations (the zero-point oscillations of the electromagnetic field), cancel about -1 per cent of the previous effect, for the heavier elements. The other lowest-order contribution, of opposite sign, is vacuum polarization. One could say that the Dirac-Fock-Breit Hamiltonian is ‘101 percent correct’ (cp. [6a]). The QED effects can be seen in accurate quantitative comparisons but have so far not led to qualitative chemical changes.

Which orbitals to use in chemistry?

The chemical behaviour of the elements in Fig. 1 is mostly driven by the orbitals, occupied in the atomic ground state, and given in the right-hand marginal. Sometimes also other orbitals, which are unoccupied in the atomic ground state but energetically accessible for bond formation, can participate. Thus we can have the predicted [11] *pre-s* Og⁻ anion, the *pre-p* Be, Mg; Zn, making bonds with their $ns + np$ orbitals, the *pre-d* Ca, Sr, Ba; Cs and the *pre-f* Th.

A recent example was the synthesis of $[\text{Ba}(\text{CO})_8]$, which fulfils an 18-electron rule by using the originally empty $5d$ shell of the central barium atom [12]. The atomic ground state does not always explain the molecular outcome. Moreover, remember that electron correlation can make the concept of electron configurations diffuse.

‘Secondary periodicity’

Biron [13] pointed out in 1915 that every second period has specific properties. Taking the Group 15 as an example, along the series (N, P, As, Sb, Bi) (Biron, p. 971), the dominant oxidation states are III, V, III, V, III, respectively. The anomaly at As can be attributed to partial screening by the filled $3d$ shell. The anomaly at Bi is due to both an analogous partial screening by the $4f$ shell and to relativistic effects [14].

Another vertical anomaly is the small radius of every atomic shell ($1s, 2p, 3d, 4f, 5g$) with a new orbital angular momentum quantum number, l . The author [15] used the name ‘primogenic repulsion’ for its effect on the higher shells. In Russian literature the term ‘kainosymmetric’ is often used for these ‘first-born’ shells [16].

The inert-pair effect

Sidgwick [17a] called attention in 1933 to a decrease of the main oxidation state by two units for 6th-period elements, take Pb(II) as an example. A first explanation would be the relativistic 6s stabilization. Closer studies involve the hybridization of the metal (6s, 6p) orbitals with the ligand np orbitals [17b].

‘False friends’

The gold atom is almost as electronegative as iodine; we can see its outermost shell as either a 6s¹ electron, or a 6s⁻¹ hole. A wide chemistry of the auride ion, Au⁻, is known [18]. For a comparison of aurides with other ‘halides’, see also [19].

Going one step left from gold, solid Cs₂Pt and other Pt^(-II) compounds were studied in the group of Jansen [20]. In molecules, in addition to σ bonding, also analogous 2p π and 5d π bonding was identified between OCO and PtCO, respectively, leading to multiple bonding [21].

In the uranyl-like isoelectronic series, OUN⁺ and OUIr⁺ were found to have similar triple bonds [22] and the latter species was later produced in mass-spectroscopy [23]. These later chemical analogies were initially unexpected.

Nuclear stability

The chemical predictions quoted here are based on theoretical, relativistic quantum chemical calculations using established electronic Hamiltonians. The nuclei are simply assumed to exist, with a realistic, finite nuclear size. The synthesis of heavier nuclei, up to E118 (Oganesson), is demanding. The most recent nuclear syntheses were completed in a friendly collaboration between laboratories in Oak Ridge and Dubna. The lifetimes of these nuclides are short; for example, the present Og isotopes have lifetimes below a millisecond. The most challenging production bottleneck is, however, not the short lifetime but the small nucleosynthetic cross-section for these elements. If the experiment runs for a year and yields less than a handful of desired product nuclei, this creates an obvious problem, even with nearly 4 π detection (all scattering directions seen) and an almost noiseless apparatus. The current situation on superheavy elements is discussed by Giuliani et al. [24].

A quantum chemist can always assume a finite nucleus of realistic size for any $Z < 173$ and do *ab initio* calculations for that theoretical model, whether or not such nuclei or their compounds are ever made. One even could claim that some general conclusions could possibly be drawn, such as the possible existence of a 5g series or the vast spin-orbit effects.

In defence of the current PT: what are the choices?

Figure 1 illustrates a recent choice of IUPAC PT layout (highlighted in yellow). Note the placement of all lanthanides and actinides in Group 3. One could, however argue certain points:

- H is now in Group 1, because it is often manifested as H⁺, or neutral. If an emphasis was placed on hydrides (H⁻), one could argue for having hydrogen also in Group 17.
- The noble gas He is now in Group 18 with the other noble gases. Apart from spectroscopic species, like the astrophysical, diatomic HeH⁺, or high-pressure compounds, like Na₂He [25], helium is still a very noble gas. As stressed by the authors, this compound is a sodium electricle containing He(0). If one would like to emphasize heliums 1s² electronic structure, one could also have it in Group 2. Its chemical behaviour is, however, not that of an alkaline earth. Note the easy ns-np-(n-1)d hybridization among heavier Group-2 elements, lacking for helium.

- (c) How long f-element rows? One now has a 15-element lanthanide (Ln) row from La to Lu. All of these elements are (mostly) trivalent. Their ionic radii or ionization potentials exhibit a systematic relationship along the series. It is entirely plausible to count from $4f^0$ to $4f^{14}$, and to leave a hole in Group 3 of Period 6. Moreover this completely avoids the heated argument on which end should one cut off – La or Lu. A clear advantage is then having all these, mostly trivalent, rare earths in the single Group 3, corresponding to three valence electrons.
- (d) Impressive experiments and computations [26] have recently verified that a free Lr atom has a $7s^27p^1$ configuration, different from the $6s^25d^1$ for a Lu atom. Computations for a handful of *molecules*, however, find a complete analogy between Lu and Lr [27], see Fig. 2. That said, if our PT is to be driven by chemistry, there are no reasons to change Fig. 1.
- (e) The 32-column option? Some desirable properties of a PT could be:
1. The column (or ‘Group’) number g (or $g-10$) is the maximum number of valence electrons. The oxidation state is then the same number or, counting holes in the spirit of Abegg’s contravalance [29], the negative number, $g-18$.
 2. The valence atomic orbitals along a row are constant in a block and equal to those in the right-hand margin.
 3. The nuclear charge, Z , increases systematically towards right.
 4. The shape should be typographically convenient.

Of these properties, Fig. 1 fulfils 1, 2 and 4 but violates 3 for certain superheavy elements when relativistic effects so require. Conversely, the 32-column ‘long-form’ PT favoured by Scerri [30] (see his Fig. 1) violates (1) by having very many potentially Group-3 columns and may also violate (4). It does satisfy (3).

The ‘Madelung rule’

The order of filling shells in a neutral atom is approximately the one given in Fig. 3. It was extended to $Z=172$ in [4]. This mnemonic device is usually called the Madelung or $(n+l, n)$ rule [31], although its shape appears to be first presented by Janet [32a] or actually Sommerfeld [32c].

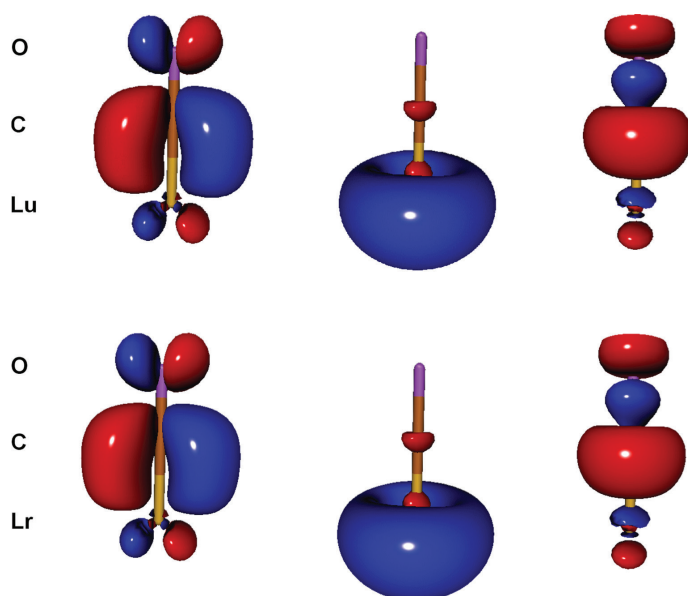


Fig. 2: The valence molecular orbitals (MO) of theoretical LuCO and LrCO molecules [27]. Note the similarity. The LuCO is experimentally known, see [28]. As discussed there, the main Ln bonding orbitals are the 6s and 5d. The MO:s from left to right are the M–C pi bond (a donation from M to the CO pi* MO), a sigma lone pair, and the M–C sigma bond. The similarity between Lu and Lr is not a mistake, but the message.

The ‘Madelung rule’ up to $Z = 172$

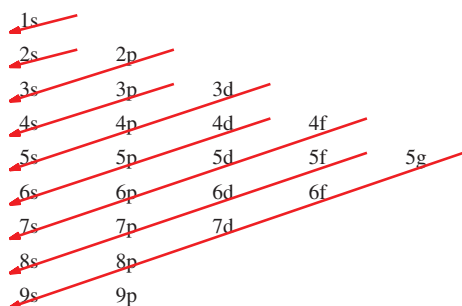


Fig. 3: The ‘Madelung rule’ for filling atomic orbitals up to $Z=172$, corresponding to Fig. 1 (reproduced from Pyykkö [4]).

Models for reproducing the PT

How to explain this approximate order of level filling in neutral, or nearly neutral atoms? For an electron in a Coulomb field, each new n introduces a new l_{\max} and this degeneracy of all levels with the same n was discussed by Fock [33] using momentum-space wave functions in a four-dimensional space. Ostrovsky [34] used coordinate space.

Concerning the physics of many-electron atoms, the Dirac-Fock-Breit (DFB) Hamiltonian, supplemented with some estimate of leading quantum electrodynamic (QED) effects, gives an excellent description. As an example, Pašteka et al. [35] calculated the ionization potential and electron affinity of a gold atom with milli-electronvolt (meV) accuracy. The bottleneck rather was in the handling of electron correlation. Coupled-cluster methods with up to pentuple excitations were used. Thus no surprises are expected here. Atoms follow Physics.

A much simpler task is the question of the filling order of one-electron levels in some effective-potential model for a many-electron atom, such as a Thomas-Fermi one. This has been tried since Fermi [36] or Goepert Mayer [37], and various versions have been included in textbooks, such as Sommerfeld [38], Gombás [39], or Landau and Lifshitz [40]. Some examples on these studies are [41, 42]. The predictions for filling new shells are quite similar, see Table 1. In a screened-Coulomb potential, the attraction must be sufficient to balance the centrifugal potential for l . This type of reasoning was used by Goepert Mayer [37] to discuss the Z where $4f$ and $5f$ states are first occupied. For reviews see Ostrovsky below. The T–F treatment yields the Z values for a new l at

$$Z = 0.17 (2l + 1)^3 \quad (1)$$

with the pre-coefficient chosen by Landau and Lifshitz [40]. The results in Table 1 are in a surprisingly close agreement with more exact results. Note that the T–F potential is just one of the various screened-Coulomb potentials, which do the job. The literature on which T–F potential at which Z starts a given l is broad, see Table 1. Essén [43] gives for filling the first state of l the nuclear charge

Table 1: The first nuclear charges, Z , where the atomic orbitals l are occupied for a Schrödinger equation in a Thomas-Fermi potential (from Fermi [36], Goepert Mayer [37], Iwanenko and Larin [41], Landau and Lifshitz [39] [present eq. (1)], Essén [43]) and from Dirac-Fock-level relativistic calculations [3].

l	Fermi [36]	Goepert [37]	Iwanenko [41]	Landau [39]	Essén [43]	DF [3]
1	5		5	5	5	5
2	21		22	21	21	21
3	$\geq 55, 58$	$\geq 57; \geq 91$	58	58	57	58
4				124	121	125

$$Z(l) = 2 \left(\sum_{n=0}^l 2n^2 \right) + 1 \quad (2)$$

The doubling of periods with two periods of lengths 8, 18 and 32 each has been noticed by many authors, Löwdin [44], Demkov and Ostrovsky [45], Odabasi [46], Ostrovsky [47], Essén [43], Katriel [48], Kitagawara and Barut [49], Novaro [50] and Kibler [51] have discussed possible underlying dynamical symmetries. An alternative is that there is no deep symmetry reason and that one only needs the quoted ‘nuts and bolts’ of the DFB Hamiltonian.

For later reviews on the doubling question, see Ostrovsky [52].

Concluding, of the existing literature on the PT, we would still like to remind the reader of the articles by Schwarz [53–55] and of a factor-analytical search for chemical similarities by Leal and Restrepo [56].

Did our department contribute to the story?

The new Chemical Laboratory building of the old Kungliga Åbo Akademi (our direct legal predecessor before the removal from Turku to Helsinki in 1828) was inaugurated on 13 April 1764 under Professor Pehr Gadd. The 250th anniversary was celebrated in 2014 by having business as usual.

Gadd’s successor, Johan Gadolin (1760–1852) [57] published the first chemical analysis of a black mineral from Ytterby (near Stockholm) in 1794 (German version published in 1796). The paper was translated to modern chemical terminology by Pyykkö and Orama [58].

Starting from this mineral, which was essentially $\text{FeBe}_2\text{Y}_2\text{Si}_2\text{O}_{10}$, he obtained a new ‘earth’, i.e. oxide, essentially Y_2O_3 , possibly with traces of other rare earths. The mineral was later named *gadolinite*. Although one cannot necessarily claim that Gadolin found a specific element, he did contribute to finding an entire family of 16 elements. Organizing these kept chemists busy for another century. In 1886 one of them was given the name *gadolinium* (*Gd*).

Circumstantial evidence from the parallel case of samarium (*Sm*) by the same authors suggests that Lecoq de Boisbaudran and Marignac considered both the mineral and the eponym, or the person behind its name. For more details on *Gd*, see [59] and supplements to it. In 1994 a bicentennial conference, 2-ICFE, was held in Helsinki, with a conference excursion to Ytterby, see Fig. 4.

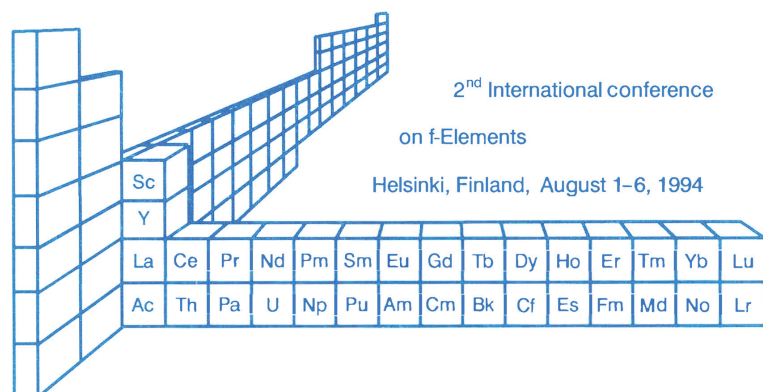


Fig. 4: In 1994 an International Conference on f-Elements was held in Helsinki to celebrate the bicentennial of Johan Gadolin’s 1794 analysis [57]².

² An earlier version of the present article was published also in the 2019 brochure Chemistry News of the author’s Department.

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Graphical abstract

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An essay on periodic tables

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Conference paper: A possible arrangement of the elements 119–172 is suggested, based on atomic, ionic, and molecular calculations. Certain trends among the experimentally known elements 1–118 are discussed.

Keywords: analogies between elements; chemical bonding; lanthanides; Mendeleev 150; periodic tables; secondary periodicity; superheavy elements.

1	H	2											13	14	15	16	17	2	Is		
2	3	4											5	6	7	8	9	10	2s2p		
3	11	12	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	3s3p		
4	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	4s4d4p		
5	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	5s4d5p		
6	55	56	57	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86	6s5d6p		
7	87	88	89	104	105	106	107	108	109	110	111	112	113	114	115	116	117	118	7s6d7p		
8	119	120	121	122	123	124	125	126	127	128	129	130	131	132	133	134	135	136	137	138	8s7d8p
9	165	166	167	168																9sp	
6	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71					4f	
7	89	90	91	92	93	94	95	96	97	98	99	100	101	102	103					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