

Atomic Core Based Periodic System of Elements. A Contradictory Approach to the Arbitrary 1–18 Group Numbering in the Long Form of Atom Based Periodic System

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Problems connected with the long version of atom-based Periodic System of chemical elements with arbitrary 1–18 group numbering recommended by IUPAC are discussed. Introducing the atomic cores of elements instead of atoms to the Periodic Table enables to define unequivocally the Periodic System as a triparametric classification resulting from three numbers: the number of core electron shells n , the core charge q , and the number of valence subshells l . The core based periodic chart is free of any imperfections and limitations of the atom based system and it enables reasonable numeration of groups and periods according to the nql parameters.

Key words: Periodic System of elements, atomic core, elements classification

The Periodic System of elements is based on parameters originating from the classified objects [1] and its interpretation evolves, almost permanently, since its creation in 1869 up to now, in order to keep pace with the increasing knowledge on the structure of matter [2]. However, nowadays the interpretation of the Periodic Chart seems to be too conservative. A number of new facts concerning chemical elements have passed by the Periodic System despite of the fact that they were connected with its proper understanding. The actual state of interpretation of the Periodic System of elements and its imperfections will be discussed in relation to the actual long form, recommended by IUPAC (Figure 1) [3], starting with some problems not resolved for years.

The chemical inertness of the atoms of noble gases has been a basis of the particular role they play in the Periodic System. Under these circumstances the synthesis of some compounds of noble gases has become a sort of a revolutionary event, which nevertheless has passed, by the Periodic System without any consequence that would approach the System to the new experimental reality.

About a half century ago it has been noticed that stable electronic structures, but different from those existing in the noble gases (with 8 electrons in the outer electron shell), are observed also in the divalent cations of zinc, cadmium and mercury (with 18 electrons in the outer shell). No relation has been conceived, however, between this observation and the Periodic System, in which the arrangement has been confined to neutral atoms, not to ions. As a result, the observation has lost its

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significance and fell into oblivion. It was not commonly known, that a similar role is played also by trivalent cations of lutetium and lawrencium (with $32 + 8$ electrons in outer shells) [4].

An important classification problem, persisting for many years and not yet satisfactorily resolved, is connected with the position of hydrogen and helium in the Periodic System. As generally known, the properties of hydrogen do not correspond to those of elements of either group one, where it has been usually located, or group seven, where it was occasionally placed. Acquiescently hydrogen is sometimes treated as an element outside the group classification. There is no serious doubt, however, concerning the position of helium in the eight main group (in IUPAC version the eighteenth), although it neglects the strong relations of He with hydrogen, both from the genetic and structural viewpoints. Only in some exceptional cases helium was located in a separate position, along with hydrogen (*e.g.* in Bohr version of Periodic System [5]) as well in separate block 1 s.

The positions of hydrogen and helium are not the only doubts connected with the classification of elements. The problem of proper interpretation of the Periodic System in the region of the second group is confused by regarding zinc, cadmium, and mercury as transition elements despite of the fact that they are, in reality, the main group elements as having the *d* sub-shell completed with 10 electrons (as it has been pointed out by many authors). The assignment of the zinc group elements to the transition group has been forced by the placement of the calcium group elements in the second main group.

Some incoherences of the classification of atoms based on its electron structures also exist in the block allocation of Cu, Ag, Au, and Uuu. From formal reasons it might be possible to put them into the main groups block taking into account their $d^{10}s^1$ electron structure.

No success has been achieved in considerations, in the first half of the 20th century, on the limits of the Periodic System [6]. The investigation concerned mainly the lower limit of the System expected to be a zero period, a two-element analogue for the first period of elements: H–He. Also the upper boundary of the Periodic System was a subject of considerations long ago, prior to the discovery of the trans-uranium elements, when uranium was the last element known and the structure of the end of the seventh period remained unexplored.

The lack of satisfactory comprehension for a triparametric, hence tridimensional nature of the Periodic System, which has been anticipated almost since the time of Mendeleev's activity [7], was one of the reasons of creation of a diversity of versions of the System. Under these circumstances some inconsequences appeared in the digital description of the periodic system, in particular in the numbering of the groups of elements. The numbering of the groups was particularly inconsequent in the long version of the periodic system. In 1964 Ölander [8] proposed to systematise the numbering of groups in this version by assigning the numbers from 1 to 18 to successive groups of elements. Because of the lack of relationship between the numbering of the groups and the parameters describing the elements that idea found no approbation and soon it was abandoned. Ölander's numeration has been revived in

the eighties by the IUPAC Commission of Nomenclature in Inorganic Chemistry (CNIC) [8], for the reasons known only to this body, then accepted and generally recommended as a standard [3,9] (Fig. 1), despite of the critical remarks presented by many individuals and organisations [15].

It should be stressed that the group analogies are mainly stoichiometric [1], while the periodic ones are mainly structural [10]. Lately, the topic interest in the utilisation of the Periodic Table shifts from the relationships inside the groups to those existing in the periods. In this situation the numbering of the groups and sub-groups (in the long form related to as the groups) in the Periodic Table is to be considered only jointly with the numeration of the periods and sub-periods, what is not possible in the long form of the Periodic Table which, contrary to the short form, takes no account of numerical differentiation of main and transition elements in a period.

The recommended by IUPAC direct numeration of the groups according to their succession in the long form of the Periodic Table (Fig. 1) destroys the essence of the classification as determined by digital parameters of the classified objects. The numbering of groups of elements in the periods 1, 2, and 3 has no relation with the digital parameters of these elements. Hydrogen is placed in the group 1, but its nearest neighbour helium has been located in the group 18. No parameter of helium can justify its assignment to the group 18. In the second period lithium and beryllium are placed in the groups 1 and 2, but the following series of elements: boron, carbon, nitrogen, oxygen, fluorine and neon have been located in the groups 13, 14, 15, 16, 17 and 18. In the same manner in the third period sodium and magnesium remain in the groups 1 and 2, but the elements that follow them in the period (*i.e.* aluminium, silicon, ..., argon) have been located in the groups 13–18. It is possible to understand this numeration in periods 4 and 5, but again not in 6 and 7 because of the presence of *f* elements. (see Fig. 1).

1																	18	
H																	He	
2	3	4											5	6	7	8	9	10
Li	Be											B	C	N	O	F	Ne	
11	12											13	14	15	16	17	18	
Na	Mg											Al	Si	P	S	Cl	Ar	
19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr	
37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe	
55	56	57-	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86	
Cs	Ba	71	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn	
87	88	89-	104	105	106	107	108	109	110	111	112	113	114	115	116	117	118	
Fr	Ra	103	Rf	Db	Sg	Bh	Hs	Mt	Ds	Uuu	Uub	Uut	Uuq	Uup	Uuh	Uus	Uuo	
Lanthanide series		57	58	59	60	61	62	63	64	65	66	67	68	69	70	71		
		La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu		
Actinide series		89	90	91	92	93	94	95	96	97	98	99	100	101	102	103		
		Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr		

Figure 1. Long version of periodic chart with 1–18 group numeration according to IUPAC recommendation [3].

DISCUSSION

In the middle of the XX century there appeared, in the course of studies on the structure of solid metallic phases, a concept of atomic core as a repeatable, positively charged particles determining the nodes of crystal lattice, linked together by means of delocalised electrons. In the nineteen sixties the concept of atomic core has been adopted for use in the description of chemical structures and was defined as positive charged system of atomic nucleus with complete electron shells resulting from elimination of all valency sphere electrons of the atom [11,12]. In analogy to the nuclides it has been proposed to refer to these particles as the “corides”.

The replacement of neutral atoms by atomic cores in the Periodic System has revealed its tri-dimensional nature described by three numerical classification parameters [4,12], namely:

1. The number of the core electron shells n defining the period in the Periodic System (lesser by one from the number of the atom electron shells):

0(-) 1(K) 2(KL) 3(KLM) 4(KLMN) 5(KLMNO) 6(KLMNOP)

2. The core charge q which defines the group in the System from 1+ to 16+.
3. The number (and sequence) of vacant valency electron sub-shells l which defines the blocks of elements:

1 (*s*) 2(*sp*) 3(*dsp*) 4(*fdsp*)

The classification space is determined by three discrete axes n , q and l that can assume then the following integers:

n : 0, 1, ..., 8

q : 1, 2, ..., 16

l : 1, 2, 3, 4

In the case of a rectangular system of axes n , q and l the classification space is divided, according to the corresponding discrete values, into cubic cells in which are located the cores of chemical elements (Figure 2).

The discrete nature of the classification axes makes it possible to represent the tridimensional system graphically on a plane in a number of ways. The simplest one is to divide the third and the shortest axis l into square cells determined by individual

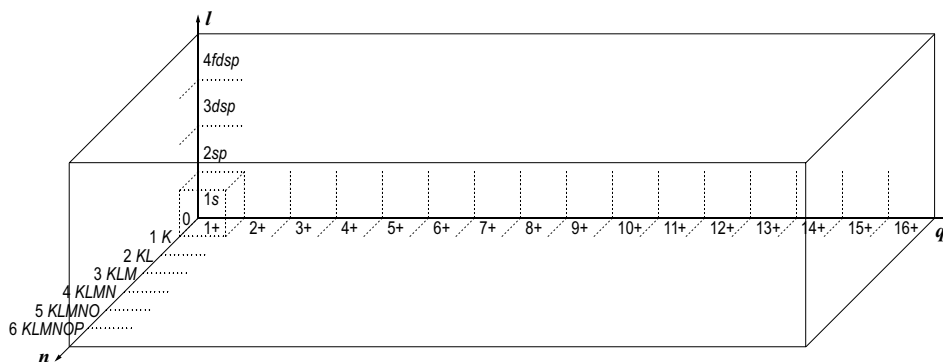


Figure 2. Orthogonal coordinates of triparametric core-based Periodic System of chemical elements, where: q – core charge, n – number of core shells, l – number of valence sub-shells.

values of n and q and to dispose them along the diagonals of the cells, as shown in Figure 3. This version is related with popular in the middle of the past century short

n	c_s	v_s										l																
		0	1+	2+	3+	4+	5+	6+	7+	8+	9+		10+	11+														
0			$1s$	$2s$	$2p$	$3s$	$3p$	$3d$	$4s$	$4p$	$4d$	$4f$	$5s$	$5p$	$5d$	$5f$	$6s$	$6p$	$6d$	$6f$	$7s$	$7p$	$7d$	$7f$	$8s$	$8p$	$8d$	$8f$
1	$1s$		$2s$	$2p$	$3s$	$3p$	$3d$	$4s$	$4p$	$4d$	$4f$	$5s$	$5p$	$5d$	$5f$	$6s$	$6p$	$6d$	$6f$	$7s$	$7p$	$7d$	$7f$	$8s$	$8p$	$8d$	$8f$	
2	$1s, 2s$		$2s$	$2p$	$3s$	$3p$	$3d$	$4s$	$4p$	$4d$	$4f$	$5s$	$5p$	$5d$	$5f$	$6s$	$6p$	$6d$	$6f$	$7s$	$7p$	$7d$	$7f$	$8s$	$8p$	$8d$	$8f$	
3	$1s, 2s, 2p$		$2s$	$2p$	$3s$	$3p$	$3d$	$4s$	$4p$	$4d$	$4f$	$5s$	$5p$	$5d$	$5f$	$6s$	$6p$	$6d$	$6f$	$7s$	$7p$	$7d$	$7f$	$8s$	$8p$	$8d$	$8f$	
4	$1s, 2s, 2p, 3s$		$2s$	$2p$	$3s$	$3p$	$3d$	$4s$	$4p$	$4d$	$4f$	$5s$	$5p$	$5d$	$5f$	$6s$	$6p$	$6d$	$6f$	$7s$	$7p$	$7d$	$7f$	$8s$	$8p$	$8d$	$8f$	
5	$1s, 2s, 2p, 3s, 3p$		$2s$	$2p$	$3s$	$3p$	$3d$	$4s$	$4p$	$4d$	$4f$	$5s$	$5p$	$5d$	$5f$	$6s$	$6p$	$6d$	$6f$	$7s$	$7p$	$7d$	$7f$	$8s$	$8p$	$8d$	$8f$	
6	$1s, 2s, 2p, 3s, 3p, 3d$		$2s$	$2p$	$3s$	$3p$	$3d$	$4s$	$4p$	$4d$	$4f$	$5s$	$5p$	$5d$	$5f$	$6s$	$6p$	$6d$	$6f$	$7s$	$7p$	$7d$	$7f$	$8s$	$8p$	$8d$	$8f$	

Figure 3. Planar version of triparametric periodic chart of atomic cores with / axis splitted into diagonals of particular $n-q$ square cells. Core shells and valence sub-shells are marked as c_s and v_s , respectively.

form of Periodic Table. Another way of representing the tridimensional classification on a plane might be based on a block system, in which the particular blocks are cross-sections determined by constant values of l (Fig. 4). That version is in some relation to Werner's long Periodic Chart [13] with separate blocks of elements but it results from digital parameters of classified objects (cores) and is free of the group numbering difficulties.

The atomic number, which is still considered to be the essential parameter of the Periodic System of atoms of elements, becomes a parameter of another system – the classification of nuclides – conforming to the number of protons and neutrons. It should be stressed that the atomic number, which is a base for the definition of the chemical element, is not a parameter determining the Periodic System of cores of chemical elements. It has been related only with the history of creation of the Periodic System of atoms of chemical elements and with its interpretation.

1 s	0	1	2	$q \rightarrow$															
		H	He																
2 sp	1	3	4	5	6	7	8	$q \rightarrow$											
		Li	Be	B	C	N	O	F	Ne										
	2	11	12	13	14	15	16	17	18										
		Na	Mg	Al	Si	P	S	Cl	Ar										
	3		30	31	32	33	34	35	36										
			Zn	Ga	Ge	As	Se	Br	Kr										
	4		48	49	50	51	52	53	54										
		Cd	In	Sn	Sb	Te	I	Xe											
5		80	81	82	83	84	85	86											
		Hg	Tl	Pb	Bi	Po	At	Rn											
6		112	113	114	115	116	117	118											
		Uub	Uut	Uuq	Uup	Uuh	Uus	Uuo											
3 dsp	3	19	20	21	22	23	24	25	26	27	28	29	$q \rightarrow$						
		K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu							
	4	37	38	39	40	41	42	43	44	45	46	47							
		Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag							
	5			71	72	73	74	75	76	77	78	79							
			Lu	Hf	Ta	W	Re	Os	Ir	Pt	Au								
6			103	104	105	106	107	108	109	110	111								
			Lr	Rf	Db	Sg	Bh	Hs	Mt	Ds	Uuu								
4 fdsp	5	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	$q \rightarrow$	
		Cs	Ba	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb		
	6	87	88	89	90	91	92	93	94	95	96	97	98	99	100	101	102		
	Fr	Ra	Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No			

Figure 4. The block version of triparametric periodic chart of atomic cores.

In the Periodic System of cores of elements each atomic core is unequivocally identified by the three numbers: n , q , and l . By suppressing the variations of individual classification parameters one can obtain definite ordered sets of the cores:

$n = \text{const}$ – a Period of elements (distinguished with capital letter P),

$q = \text{const}$ – a Group of elements (distinguished with capital letter G),

$l = \text{const}$ – a block of elements,

$n = \text{const}, l = \text{const}$ – a period in a block of elements (a sub-period),

$q = \text{const}, l = \text{const}$ – a group in a block of elements.

The sixth combination possible: $n = \text{const}, q = \text{const}$ has not been taken into consideration as it can comprise only very short series of elements (three elements at the utmost). Obviously, putting the values of $n = \text{const}, q = \text{const}$, and $l = \text{const}$ reduces the System to a single element.

The electronic structures of the atoms of noble gases, whose canonic nature in the Periodic System has been undermined by the valence nature of their outer electron octet, appear in the core Periodic System as the canon structures of monovalent cores of elements following the noble gases: $\text{Li}^+, \text{Na}^+, \text{K}^+, \text{Rb}^+, \text{Cs}^+, \text{Fr}^+$. Beside, there appear in the core system canon structures of divalent cores $\text{Zn}^{2+}, \text{Cd}^{2+}$ and Hg^{2+} and trivalent cores Lu^{3+} and Lr^{3+} . Passing over the electronless core of hydrogen we have up to 12 canon electronic structures of atomic cores of above mentioned elements opening particular periods in blocks, that are then replicated by the elements that succeed them in the period in the given block, with increasing core charge (see Fig. 3) [14].

Some interesting consequences result from the division into blocks of elements, which is different in the core version of the Periodic System. Namely, they do not result from the distribution of valency electrons in the atom, but from the number of valency sub-shells. In the system defined in this way the block s consists of only two elements, hydrogen and helium, so much different from all the other elements. It seems that these new, univocally determined positions of hydrogen and helium resolve ultimately the difficulties connected with their location in the Periodic System.

The new, block arrangement is capable to resolve the classification difficulties of elements of the second Group. It has appeared now, that the block sp comprises beryllium, magnesium, zinc, cadmium, mercury, and ununbium whereas calcium and strontium belong to the block dsp , and barium and radium belong to the block $fdsp$. Such a grouping has enabled the re-appearance of the calcium group (alkaline earth group: Ca, Sr, Ba, Ra). A similar arrangement can now be found in the first Group of the System. Only lithium and sodium belong to the block sp , and the old potassium group comprises now potassium and rubidium from the block dsp , as well as caesium and francium from the block $fdsp$. It should be pointed out, however, that the block properties of the elements appear as far as the possibility of binding electrons by their atomic cores. For this reason they are very faint in elements with a monovalent cores, hardly observable in the elements with divalent cores, they occur in the elements with three-valent and are fully developed in those with more positive

cores. On the other hand the block properties of elements may be limited by the irreversibly bonded valence electrons which can occur by relatively high charged cores (mainly in the *fdsp* block).

Electron structures of atomic cores of elements, contrary to electron structures of neutral atoms show no deviation from general rules and thanks to that the atomic core based Periodic Chart is free from any uncertainties of atomic version.

The Periodic System of atomic cores provides a new insight into the problem of the limits of Periodic System. The lower limit of the System appears here in the form of the zero period. Contrary to the other periods it has no homologue and is unique as the border period of electronless cores. There is also an outline of the upper limit of the System. From a practical chemical viewpoint some form of a limit may be the element 118.

CONCLUSIONS

The IUPAC Nomenclature Commission considered the numbering of groups in Periodic System of Elements as a nomenclature problem and applied normal, for such a case, procedure searching for the most frequently used form of the Periodic System [8]. It has been found of course that it is the long form. It has not been noticed however, that the discontinuity of group numbering results, in this case, from the incoherence of long version of Periodic System and cannot be overcome without breaking the fundamental unity between group numbering and digital parameters of classified objects – atoms. IUPAC version breaks this relation and this is sufficient reason for its refusal. What more, the long version gives no possibility for periods numeration according to numeration of groups of elements.

Atomic core version of Periodic System of Elements represents well defined triparametric classification based on n , q , l numbers of cores. In contradiction to neutral atoms version, this version is free of any irregularities in generating classification parameters – electron structures (Fig. 3).

An unquestionable advantage of the Werner's long version of the Periodic Table, that has brought so much to its popularity, arises from the separation of the block of main group elements from that of the transition elements and leaving outside the System the inner transition elements. This procedure gives a more clear insight into the sub-groups (related as groups) of the main and transition elements. The same advantages are possessed by the block version of core based system being presentation of triparametric classification on a plane (Fig. 4).

The atomic core block version is the only version of the Periodic System with separated blocks which enables a coherent indexation of periods and groups of elements according to digital parameters n , q , and l . Assigning constant values i, j, k to parameters n, q, l , respectively, we arrive at:

iqk – i th period of k th block, where subsequent q values define the elements of the period,

njk – j th group of k th block, where subsequent n values define the elements of the group.

Periods and groups can also be defined in another coherent way using the name of a principal element, for example: “potassium period” ($n = 3, l = 3$) or “zinc period” ($n = 3, l = 2$) and “nitrogen group” ($q = 5, l = 2$) or “vanadium group” ($q = 5, l = 3$).

The Core Periodic Chart represents a classification system of objects that are in a simple relation to coordination centres, which play important role in chemical structures. Contrary to the *protons – neutrons* classification of the nuclides [15] it is a classification of structures not bound together by elementary transformations. It is possible to see chemical reactions as proceed within the valence electrons and ligands sphere of coordination centers, with no change of the central atomic cores. On relating the chemical structures with their transformations becomes possible in the classification of hierarchically higher structural objects by the description of the valency sphere of central cores in terms of suitable numerical parameters [16,17,18].

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