

NEW PERIODIC TABLE

- Why don't you change the viewpoint on the periodicity ? -

Katsuma YAGASAKI
College of Science, University of The Ryukyus
Nishihara, Okinawa 903-01, Japan

ABSTRACT

A new type of Periodic Table is proposed to look the electron configuration at sight. Some characteristic properties are discussed briefly for use of this table.

INTRODUCTION

We are familiar with such as the long range periodic table designated by IUPAC(1970) (IUPAC: International Union of Pure and Applied Chemistry). The author has been having some questions concerning about the table as follows: Why the atomic periodicity is divided into 8 families in spite that the electronic configuration of atoms is clearly understood by the quantum mechanics? Can we find the essential meaning in the 8 periodicity of the old style? Why are the atoms treated unevenly? For example the three transition metals in a narrow sense are situated within only one column, and both of the lanthanide and actinide groups consisting of 15 elements are set in two one frames, respectively. It is more fundamental to use the quantum state of *s*, *p*, *d*, and *f*, instead of subgroup of A and B. These questions come from the real electronic configuration against the old atomic formality.

My second claim for the periodic table is inconvenience for explanation of the physical or chemical property; why do the properties of the elements in the subgroup B change considerably among one group and neighbors, whereas, why are those in the subgroup A almost the same? Why does the ferromagnetism appear in special groups of iron, rare earth and actinide? The answers for all of them cannot be find from the atomic position itself in the conventional periodic table.

Because the property of elements comes from the electronic configuration of the atoms, the essential understanding of the elements shall be presented in the periodic table. In other words, periodic table means the electron configuration of

elements.

A new periodic table is introduced here, in which we can find the electron configuration directly at sight¹⁾.

A NEW PERIODIC TABLE

(1) Coordinate System of The Principal Quantum Number and The Azimuthal Quantum Number

The fact that the periodicity comes from the quantum state of electrons is known quite commonly. The quantum numbers defining the electron quantum state are indicated as follows; [1] the principal quantum number, n , [2] azimuthal quantum number, l , [3] the magnetic quantum number, m , [4] the spin quantum number, s , and [5] the radius quantum number, n' . Among them, the ones which regulate the periodicity mainly are the principal and the azimuthal quantum numbers. For a new periodic table, the principal quantum number n is taken as ordinate and the azimuthal quantum number l is taken as abscissa. Here, the principal quantum numbers $n=1, 2, 3, \dots$ are corresponding to the main electron shells as called K, L, M, ..., and azimuthal quantum numbers $l=0, 1, 2, 3, \dots$ are corresponding to the subshells of $s, p, d, f, \dots$ respectively. Hereafter, we call the azimuthal quantum numbers by the name of the subshells, s, p, d and f . Thus we give a position of an element as the quantum position of the electron which is newly added for the elements.

(2) The Periodic Groups and The Subgroups A and B

We will maintain the usual meaning of the groups and the subgroups in the new periodic table with some proofs as follows.

[Transition elements (in a narrow sense)]

Transition elements are settled in a 8 groups all together in the usual total table because of the number of electrons in s and p shells. However, we have ten electrons in d shell. In the new table, they will be divided into individual groups according to their nature; the eighth group is given for Fe, Ru and Os, the 9th group for Co, Rh and Ir and the 10th group for Ni, Pd and Pt, respectively.

[Lanthanides and Actinides]

Periodicity of lanthanide and actinide groups in the conventional table is neglected completely and only one position is given for all of them. However, their elements really have different properties, though it is a little less clear for lanthanides. The following division, 7 groups of 4th, 5th, 6th, 7th, 8th, 2nd and 3rd for each half series of them is more effective.

[Subgroups A and B]

We keep the idea of subgroup in the new table in order to comparison with the old ones in spite of the unnecessary idea. Here, we add a subgroup A' for f characters of lanthanide and actinide groups, as a new situation.

Azimuthal Quantum Number 1																							
Group sub group		0 (s)		1 (p)				2 (d)						3 (f)									
		I	II	III	IV	V		III	IV	V	VI		IV	V	VI	VII	VIII	II	III				
		(B)				(A)						(A')											
Principal Quantum Number <i>n</i>	1	(0) 1H 2He																					
	2	A	3Li 4Be	5B 6C 7N 8O 9F 10Ne																			
	3	A	11Na 12Mg	13Al 14Si 15P 16S 17Cl 18Ar				21Sc ₁ 22Ti ₂ 23V ₃ 24Cr ₅ 25Mn ₃ 26Fe ₈ 27Co ₇ 28Ni ₈															
	4	A	19K 20Ca	29Cu 30Zn				39Y ₁ 40Zr ₂ 41Nb ₄ 42Mo ₅ 43Tc ₃ 44Ru ₇ 45Rh ₈ 46Pd ₁₀						58Ce 59Pr 60Nd 61Pm 62Sm 63Eu 64Gd 65Tb 66Dy 67Ho 68Er 69Tm 70Yb 71Lu									
	5	A	37Rb 38Sr	47Ag 48Cd				57La ₁ 72Hf ₂ 73Ta ₃ 74W ₄ 75Re ₅ 76Os ₆ 77Ir ₇ 78Pt ₉						90Th 91Pa 92U 93Np 94Pu 95Am 96Cm									
	6	A	55Cs 56Ba	79Au 80Hg				89Ac ₁															
	7	A	87Fr 88Ra	81Tl 82Pb 83Bi 84Po 85At 86Rn																			

Fig. 1 New Periodic Table. Superscript on the left shoulder is atomic number. The subscript of *d* elements denotes the number of *d* electrons. For *s* elements, electrons of A subgroup fill the subshell initially and electrons of B subgroup fill again the subshell after the *d* occupation is completed, because the *s* occupied electrons have fallen into *d* subshell during *d* occupation.

(3) Groups of I_B and II_B

When occupation of a $n-d$ electron shell proceeds, one or two of the $(n+1)-s$ electron(s) fall(s) into $n-d$ shell, because the two energy levels are close and that $n-d$ level decreases when the shell is occupied halfly and fully. In this case, after the $n-d$ shell is completed the electrons are supplied again to $(n+1)-s$ shell : these electrons are called as I_B or II_B electrons. In order to express these electrons outside of d shell, we make the frame of d -related electrons extend to the s state, so that we can see the I_B and II_B electrons which exist outside of d shell. Thus we can make up the new periodic table as shown in Fig. 1.

[Examples for how to look the table]

(a) K (I_A): The characteristic electron for K is in $4s$ state. The states up to $3p$ shell are occupied and no electrons are in $3d$ shell.

(b) Cu (I_B): The characteristic electron for Cu is in $4s$ state as same as K, but $3d$ -shell occupation is completed.

(c) Sc (III_A): Up to $3p$ shells and $4s$ shell electrons are occupied completely, and $3d$ shell is now on the way to occupy: The characteristic electron is in the $3d$ shell which is the second outermost shell of the atom.

(d) Ga (III_B): All of the shells up to $4s$ shell are occupied completely. The characteristic electron is in the outermost shell of $4p$.

(e) Lanthanides: All of the inner shells than $4f$ and outer shells of $5s$ and $5p$ are occupied completely. 3 electrons in all are already in $6s$ and $5d$ shells. The characteristic electrons are in the $4f$ shell which is the third outermost shell of the atom.

THE ELECTRON CONFIGURATION

The structural feature of this table is characterized by the electron configuration of each atom. The more increases the ordinate number n , the more outer the electron of the atom situates. So we can see the electron configuration: the order of the energy levels of the shells indicated by arrows from inside to outside of the atom.

(1) Order of The Subshell Occupation

A group of the subshells with $n+1 = \text{constant}$ has almost the same energy of levels, and within the group, the shell with smaller number of n has the lower energy. This ordering is called as $n+1$ rule. We can look it easier if we put the I_B and II_B electrons into d shell as shown in Fig. 2. In this figure, the bold faced arrows running along the diagonal express the $n+1$ rule.

(2) Characteristic of Electrons in Each Subshell

[s] The s shells are always the outermost shells when they are filled. Electron occupation in A and B subshells in the s shell proceeds after the d shell of the second outermost

shell is open or completed, respectively.

		Azimuthal Quantum Number 1																	
		0 (s)		1 (p)			2 (d)					3 (f)							
		I	II	III	IV	V	III	IV	V	VI	VII	IV	V	VI	VII	VIII	II	III	
				VI	VII	0	VIII	IX	X	I	II								
Principal Quantum Number <i>n</i>	(0)																		
	1	H He																	
	2	Li Be		B C N O F Ne															
	3	Na Mg		Al Si P S Cl Ar			Sc Ti V Cr Mn Fe Co Ni Cu Zn												
	4	K Ca		Ga Ge As Se Br Kr			Y Zr Nb Mo Tc Rb Rh Pd Ag Cd					Ce Pr Nd Pm Sm Eu Gd Tb Dy Ho Er Tm Yb Lu							
	5	Rb Sr		In Sm Sb Te I Xe			La Hf Ta W Re Os Ir Pt Au Hg					Th Pa U Np Pu Am Cm							
	6	Cs Ba		Tl Pb Bi Po At Rn			Ac												
7	Fr Ra																		

Fig. 2 The order of subshell occupation. Basic order is in diagonal direction shown by the bold faced arrows. It appears as $(n+1)$ rule.

[p] The p shells is always situated at the outermost when they are filled as same as the s shells. The inert elements except for He appear when the outermost $s+p$ shells are occupied completely.

[d] Occupation to a $n-d$ shell begins after the $(n+1)-s$ shell is occupied completely, so the electrons in the d shell are not the outermost electrons. When d shell is filled up to a half (half filled) or a full (closed), the energy of d electrons decreases by fairly amount, so that the electron(s) which once situated in s shell fall(s) into the d shell. After the d shell is completed the s shell is filled again.

[f] Electrons of the 4 and 5f shells begin to fill the third

outermost shell as a starting point of the groups of $n+1=7$ and 8 inside of the completed 5 and 6-($s+p$) shells, respectively.

ELECTRON COUPLING IN A SHELL

(1) Number of State in a Shell

According to the space quantization, the magnetic quantum number m can take any integers whose absolute value is not larger than l :

$$m = -l, -(l-1), \dots, (l-1), l$$

Thus m can take $2l+1$ states for a given l . According to Pauli principle, every electron cannot occupy the same quantum state as the other one, so that only 2 electrons with different spin are allowed to be in the same quantum number m . The total number of electrons in each quantum number l is $2(2l+1)$. It should be noted that, as the electron has electric charge, its angular momentum carries a magnetic moment: each unit of angular momentum - $1h$ for orbital and $h/2$ for spin - corresponds to 1 Bohr magneton.

(2) Spin-Orbit Coupling (for one electron)

When an electron is revolving with an angular momentum around a nucleus, it is affected by magnetic field produced by the nuclear positive charge to orient the spin magnetic moment parallel to the magnetic field. As the magnetic moment is antiparallel to the angular momentum because of the negative charge of the electron, and as the orbital momentum is parallel to the magnetic field produced by the nucleus, the coupling of the spin and orbital angular momentum is antiparallel with each other.

TABLE 1

The order of occupation for the states specified by the magnetic and spin quantum numbers.

s ($l=0$)			d ($l=2$)			f ($l=3$)		
$m \backslash s$	$+\frac{1}{2}$	$-\frac{1}{2}$	$m \backslash s$	$+\frac{1}{2}$	$-\frac{1}{2}$	$m \backslash s$	$+\frac{1}{2}$	$-\frac{1}{2}$
0	1	2	2	5	6	3	7	8
			1	4	7	2	6	9
			0	3	8	1	5	10
			-1	2	9	0	4	11
			-2	1	10	-1	3	12
						-2	2	13
						-3	1	14

p ($l=1$)		
$m \backslash s$	$+\frac{1}{2}$	$-\frac{1}{2}$
1	3	4
0	2	5
-1	1	6

(3) Hund Rule

Hund rule expresses the order of occupation of quantum state in a subshell as the most stable coupling. The least energy can be obtained when they choose the minimum Coulomb and exchange energy within a way allowed by Pauli principle. Hund rule comes to as follows: [1] Make the resultant spin momentum be maximum. [2] Make the resultant orbital momentum be maximum under the condition of maximum spin. [3] The resultant spins and orbitals are antiparallel when electrons occupy less than half of the subshell and parallel when more than half. The order of occupation for the state specified by the magnetic and spin quantum numbers is tabulated in Table 1 and the resultant spin and orbital angular momentums for each subshell are shown in Figs. 3-6, respectively.

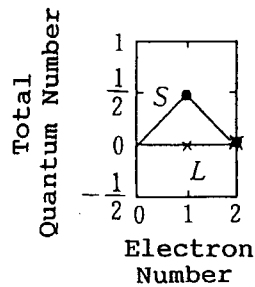


Fig. 3 The resultant spin and orbital angular momentum; $S = \sum s_i$ and $L = \sum m_i$, where i denotes i th electron. For s subshell.

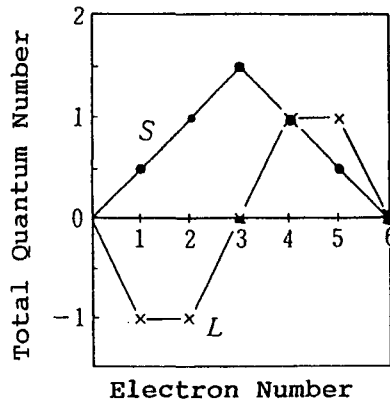


Fig. 4 The resultant spin and orbital angular momentum for p subshell.

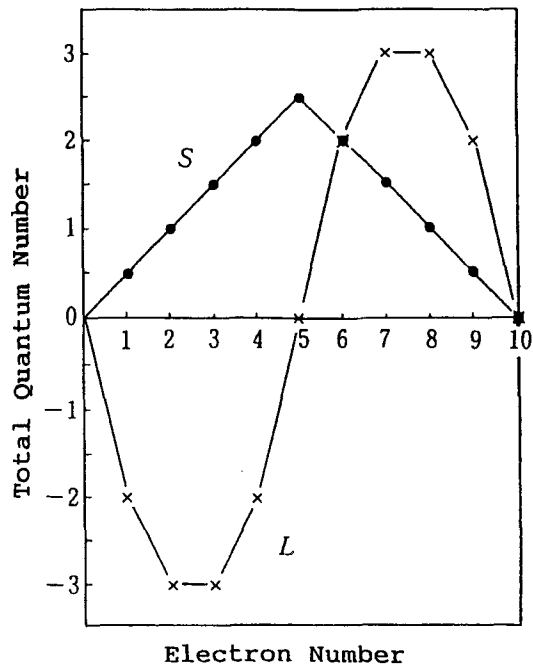


Fig. 5 The resultant spin and orbital angular momentum for d subshell.

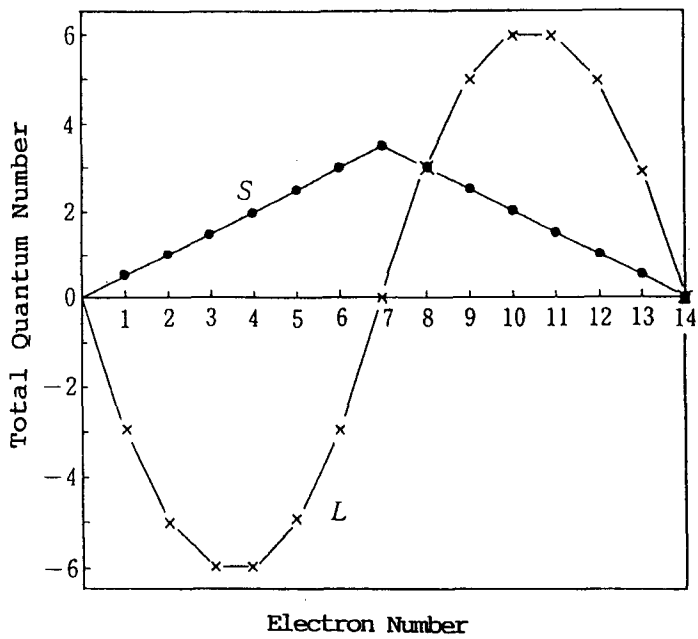


Fig. 6 The resultant spin and orbital angular momentum for f subshell.

Resultant orbital momentum becomes to be zero when the subshell is just halfly and fully occupied. The energy of the subshell takes a minimum when the orbital becomes to be zero.

ATOMIC RADIUS

Atomic radius is determined mainly by the Coulomb interaction between the coupled electrons in the outermost subshell and the nucleus. It is affected largely by screening effect of the nuclear charge with the inner side of electrons. It should be noticed that the electrons within the same subshell do not screen the nuclear charge with each other. The Coulomb attractive force between the nucleus and the outermost shell depends on number of electrons in the subshell; the force is as large as that between one positive e and one negative e when the outermost shell has only an electron, and between two positive and two negative when it has two electrons, and so on. So that the radius of the atom decreases with increasing electrons in the subshell. The atomic radius is also affected largely by the orbital angular momentum of the subshell. When an electron has large orbital angular momentum, the acceleration toward the center is very large, and this large acceleration comes from the large attractive force from the center. So that the subshell with large orbital angular momentum needs short distance from the nucleus. This is why the f subshell has a small radius. On the contrary, it should be noted that the atomic radius becomes to be enormously large

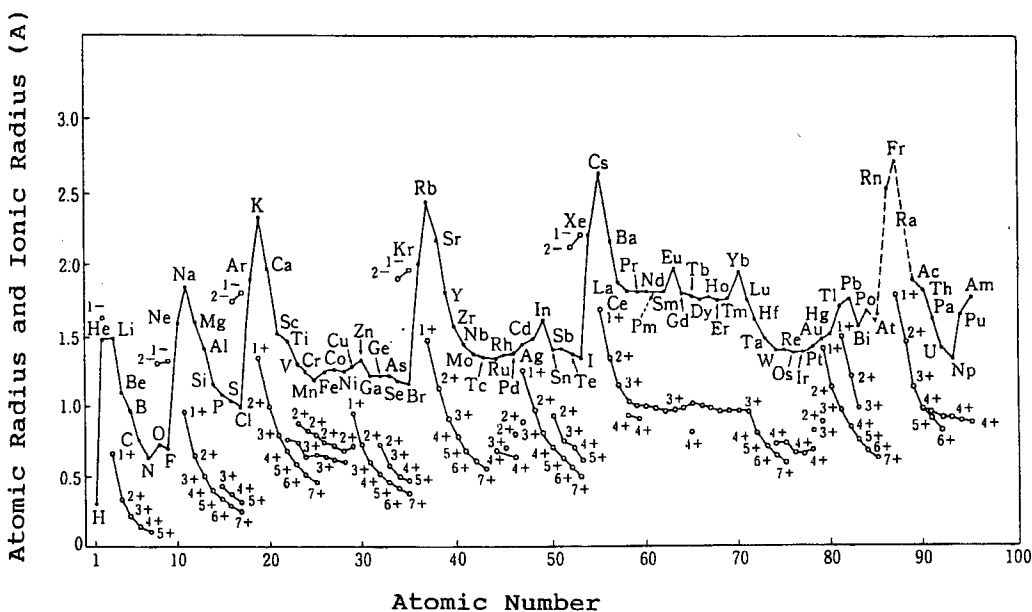


Fig. 7 Atomic (and ionic) radius against atomic number.

when the outermost shell is completely closed to make no angular momentums of orbital and spin (inert elements). As jumps in the atomic radius are occurring at the inert elements, the atomic radius as compared in a group increases with increasing the principal quantum number. The atomic radius is shown against the atomic number in Fig. 7.2)

PROPERTIES IN CONDENSED STATE

Until the former section we discussed about the property of atoms when they are each isolated. In this section we will discuss briefly about the property of the elements in condensed state (making molecules in gas, liquid or solid state). The condensation is not due to the nuclear property but due to the outermost electrons. It is very important to know the relation between the typical electrons characterizing the element itself and bonding electrons making the atoms in condensation altogether. In other words as the bonding electrons are always the outermost electrons, the property of the elements controlled mainly by the fact whether the electrons typifying the element are outermost or not.

(1) *s* and *p* Elements

The *s* and *p* elements are characterized by the outermost electrons as shown in Fig. 1. The outermost electrons are always the bonding electrons, so that the number of outermost electrons is just the number of the group to which the element belongs. This is the typical property of the *s* and *p* elements.

[Hydrogen]

The main shell with the principal quantum number $n = 1$ has only one subshell of *s*, which is completed with 2 electrons. The hydrogen atom has an electron just half of the shell. Two hydrogen atoms share their two electrons to make the shell completed, which is pretty strong covalent bonding. As these electrons are fully near their nuclei, the property of localization is very strong, and further, the mass of hydrogen nucleus is light enough, so that they make two atom-molecule not to be metallic.

[Helium]

As the 1*s* shell is closed and the electrons are fully near the nucleus, it is the most stable inert element.

[I and II group elements]

As *s* electron has no orbital momentum, the radius of the orbital is very large. Further, the radius increases with increasing the principal quantum number. It results decreasing of the localization property that comes to changing always the partner of the covalent bonding. The electrons are shared by a lot of atoms. This is called as the metallic bonding and the bonding electrons are called as conduction electrons. Bonding force of the II group elements is larger than that of the I group elements, because II group elements have two valence electrons while I group only one. The spacing of the atoms in metallic state is smaller in the II group than in the I group.

The A subgroup has a shell of inert atom just inside, accordingly it has a large atomic radius, however, the B subgroup has a completed d shell inside and a reduced atomic radius due to Coulomb interaction between the d shell and the nucleus. This results that ionization activity of A subgroup is larger than that of B subgroup.

[III_B - VII_B]

Bonding of these elements is taken place as to make number of electrons of $s+p = 0$ or 8. Covalency is the strongest in the IV_B atoms which has electrons of $s+p=4$ just half of closed shell of 8. Bonding in this element is attributed by making $s-p$ mixing orbitals. The $s-p$ mixing is the way to make bonding possibility be the largest, by promoting s electron to p orbital, which makes the strongest and most stable bonding. Among these elements, as the atomic radius decreases with decreasing n , the localizing property increases; in other words, nonmetallic property increases with decreasing n .

The element with electrons less than half of 8 has an inclination to release the excess electrons to make an ion of $s+p=0$. Bonding is attributed by these released electrons to make metallic. On the contrary, the element with electrons more than half of 8, has the opposite inclination as that less than half. They want to take electrons from each other to make $s+p$ shell complete; they becomes to be nonmetallic. The property of covalency is maximum at IV_B and decreases toward both sides. The physical property of these elements changes according to the number of bonding electrons and according to the principal quantum number, they are changing from metallic, via semimetallic to nonmetallic.

[Inert elements]

They have completed shells of outermost s and p . As they have no angular momentum, the atomic radius is extremely large.

(2) d Elements (the transition elements in a wide sense)

As we can see from Fig. 1, occupation of d shell begins after the outermost s shell is occupied. Binding force is given by the outermost s electrons in the first principle, all the d elements have almost the same bonding state. Under this condition, the d electrons are allowed to remain within the atomic position around their own nucleus without joining to bonding. Thus the magnetic moment accompanied with uncoupled electrons as shown in Table I and Fig. 5 is conserved in the condensed state (magnetic electrons). As the magnetic electrons are situated near enough with each other in the metallic state they can be exchanging to make alignment of the magnetic moments. This explanation above is rather simplified. In a real metal, as d electrons are situated at the surface of ion in metal, the locality of the d -electrons even in 3d elements are so weak compared with 4f electrons as will be described later. If the principal quantum number increases the locality is getting weaker with increasing distance from the nucleus. Thus ferromagnetism can be appeared in 3d metals only.

(3) f Elements (lanthanides and actinides)

As shown in Fig. 1, f shell is situated deep inside the

completed ($s+p$) shell. They conserve the atomic state almost completely as shown in Table I and Fig. 6 in condensed state. The role of binding is taken by outermost 3 electrons of $6s$ and $5d$ for lanthanides and $7s$ and $6d$ for actinides. Their chemical property is almost the same throughout the lanthanides. However, the periodic property of actinides are fairly strong compared with lanthanides, as the localizing property of the f electrons are considerably getting weaker. The division into groups has the real meaning for actinides. These f elements exhibit strong magnetism as well as $3d$ elements.

(4) Secondary Periodicity

Within a group, chemical and physical properties are not changing simply according to principal quantum number n . When n increases without changing symmetry of the inner shells, the property changes in a simple manner. However, non-simple changing occurs when occupation of inner d and f shells have taken place to give reduced atomic radius. This makes the secondary periodicity as shown in Fig.8.³⁾

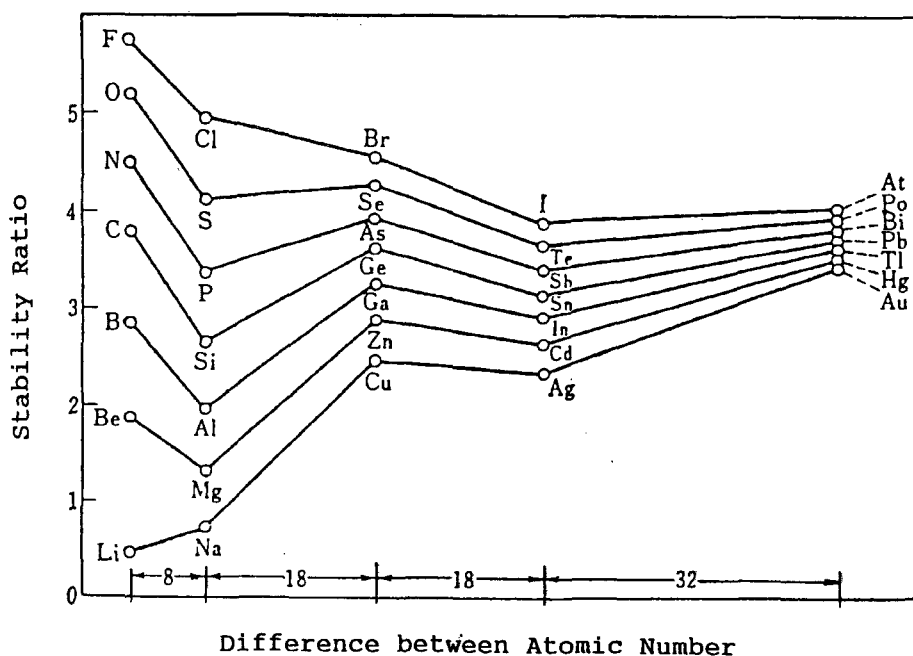


Fig. 8 The secondary periodicity for some groups. Stability ratio is taken against the difference of atomic number. Stability ratio is denoted as the ratio of the electron condensation for atoms or ions to that for the inert atom with the same number of electrons.

SUMMARY

As the periodic table is used in many ways we may have various convenient types of table according to each aiming⁴⁾. Nevertheless, it is very essential to look the electron stacking as they are in the atom, because the periodicity comes from quantum state of the electrons. Moreover, if we can look the periodicity just as their electron configuration as it is at sight of the table, the information we can get from the table increases very much to take long strides. It is the intrinsic point of this table. However, it should be noted that we neglect to show the detailed electron configuration change; for example 4s electrons during 3d occupation, and 6s5d electrons during 4f filling.

Could you try to use this table?

REFERENCES

- 1) K. Yagasaki, J. Phys. Edu. Soc. Jpn. 31(1983)49
- 2) K. Nagashima and I. Tomita, *The Periodic Table and Analytical Chemistry* Sec. 2, ed. by The Jpn. Soc. Anal. Chem. (1975, Maruzen, Tokyo) p. 28. (in Japanese)
- 3) S. Otake, *The Periodic Table and Analytical Chemistry* Sec. 2, ed. by The Jpn. Soc. Anal. Chem. (1975, Maruzen, Tokyo) p. 46. (in Japanese)
- 4) J. W. van Spronsen, *The Periodic System of Chemical Elements* (1969, Elsevier Publishing Company, Amsterdam) p. 1.