

Beyond the Madelung-Klechkowski Rule of *aufbau* Orbital Filling Principle

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Abstract We propose a more general wording for Madelung rule using a new descriptor based on the four quantum numbers n , ℓ , m_ℓ , m_s of the most recently added electron notes $K_{(Z)X}$. By this formulation, $K_{(Z)X}$ will increment as the atomic number Z increases. No exceptions will remain. It can be connected to the first ionization energy.

Keywords: Pauli principle, Madelung-Klechkowski and Hund rules, *aufbau* principle

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1. Introduction

The determination of atomic ground state electronic configuration is a fundamental knowledge and a basic concept for understanding atomic principles of matter. Electronic configuration concept is a consequence of the orbital approximation. Experimental determination of ground state electronic configuration is mainly based on the interpretation of atomic electronic spectra. Some rules can be used to find the electronic configuration of atomic ground state. They are usually named as *aufbau* (or building-up principle) from the German word meaning "construction". The filling rules are a pillar of the scientific training of students. Their success is partly the consequence of their simple statement, presentation and use. It is obvious that any reader of this paper knows all their details. However those rules remain approximate to the extent that a chemical element in five has an experimental electronic configuration that does not comply with these rules. In reality, as Löwdin [1] has claimed it, they are empirical in nature and they never been derived from quantum mechanics. The principal rule of *aufbau* principal was known as the $(n+\ell, n)$ rule. It consists of two parts: i) For neutral atoms, the electron shells fill up in the order of the quantum number sum $(n+\ell)$, ii) For electrons having equal values of $(n + \ell)$, the filling order goes with increasing n .

The authorship of this rule is still debated [2]. Written documents explicitly mention the date 1930 [3,4] but the periodic table published in 1928 by Janet [5] was using the sum $(n + \ell)$ to arrange the atoms into lines. However Goudsmith indicated that Madelung has told to him in a letter in 1926 about this discovery. Thus, it bears the name Madelung's rule [6] in Anglo-Saxon countries. But it is known as Klechkowski's rule in francophone and East European countries since it received its first theoretical justification for his work from 1951 [7,8,9]. We will use the two nomenclatures in same time. With Hund's rule

[10,11,12] and Pauli's exclusion principle[13], the Madelung-Klechkowski rule is one of the basic tools for predicting the filling of atomic orbitals.

The theoretical justification of this rule [14] is more complicated than its common form. Analytical solution to Fermi-Thomas model [15,16] using Tietz's approximation [17] leads to access to the total electrons number of one atom ${}_Z X$ by means of the equation (1)

$$N_\ell(Z) = 2(2\ell + 1) \left\{ (6Z)^{1/3} - (2\ell + 1) \right\} \quad (1)$$

According to the approximate equation (2), the quantum numbers n and ℓ depend on Z .

$$n + \ell = (6Z)^{1/3} \quad (2)$$

This paper is aimed to propose another empirical formula, easy in use, which enables us to find the true ground state electronic configuration for all atoms. In fact, we will try to give a quantitative expression to the three used rules in the determination of electronic configuration.

2. Results and Discussion

Let us begin by analyzing qualitatively the rules that lead to determining the ground state atomic configuration. The concept of electronic configuration is an offshoot of the orbital approximation which considers that it is possible to declare the poly-electrons wave function as a product of one-electron wave functions that are called orbitals. The *aufbau* orbital filling principle is based on the Madelung-Klechkowski rule that uses the sum of the principal and secondary quantum numbers $(n+\ell)$ as criterion to select the filling order of sub-shells.

The Madelung-Klechkowski rule applies in two stages: i) For neutral atoms, the electron shells fill up in the order of the quantum number sum $(n + \ell)$. ii) For electrons having equal values of $(n + \ell)$, the filling order goes with increasing n . This rule is one of those generate a maxi-

minimizing operation because it operates in ascending order of the sum $(n+\ell)$ but minimizes the value of n in case of equal value $(n+\ell)$. We could merge these two steps by making asymmetric weighting on n and ℓ . We will give a smaller coefficient to ℓ . Simply, we can test $a_1=1$ and $a_2=0.75$ obtaining the term $(n + \frac{3}{4} \ell)$. Between changing a

period with $((n+1)+\ell)$ and changing a sub-shell according to $(n+(\ell+1))$ we have not to choice because we have two different values which are $(n+1+0.75 \ell)$ and $(n+0.75 \ell+0.75)$. The smallest of them corresponds to the period with the smallest value of n . Figure 1 shows the variation of $(n+\ell)$ and $(n+0.75 \ell)$ versus the atomic number Z . Corresponding values are gathered in Table 1.

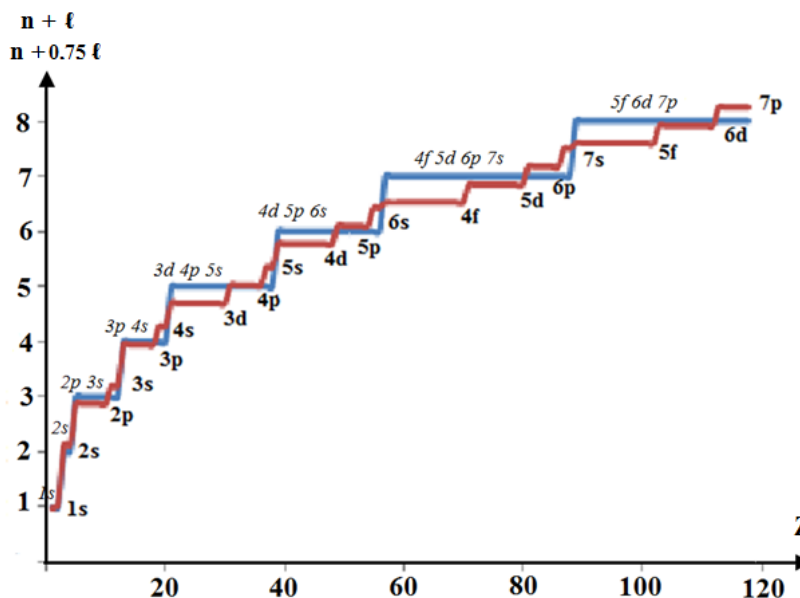


Figure 1. Variation of $(n+\ell)$ and $(n+0.75\ell)$ versus the atomic number Z

In both cases we are dealing with bearings curves. With the traditional rule, each level is relative to all sub-shells of the same amount $(n+\ell)$. However, in that we propose,

each level corresponds to a different sub-shell and their order totally respect that obtained by conventional application of the Madelung-Klechkowski rule.

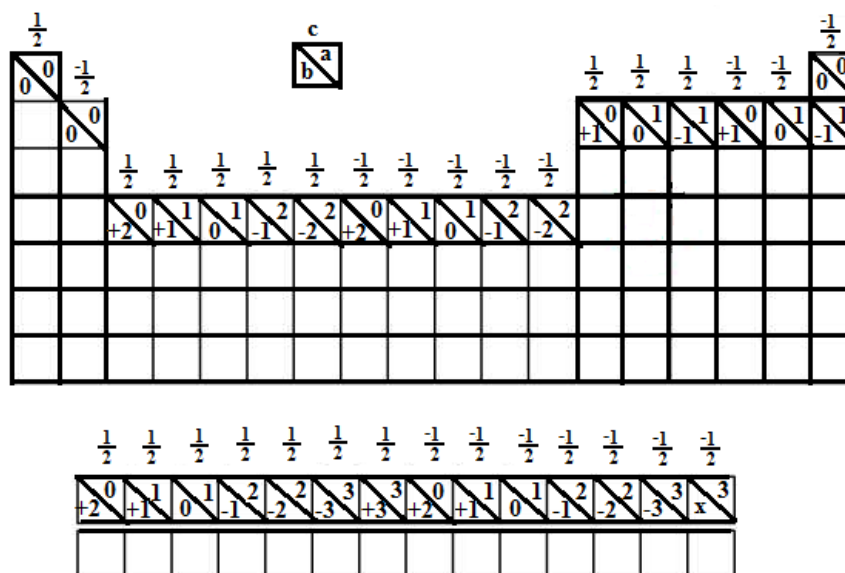


Figure 2. Distribution of quantum number m_l . In each case the top value (a) corresponds to this work, the bottom (b) the one proposed by Strong [18] and the top of the box (c) is m_s

Let us now deal with Hund' rules. They involve implicitly the magnetic quantum number m_l forcing sub-shell electrons for distribution on different orbital and explicitly the spin quantum number m_s because the electrons are bound to keep up the same spin states. The intervention of the magnetic quantum number is of implicit use because no number is attributed to a specific orbital of the sub-shell. However, some rare periodic tables allow the quantum numbers m_l and m_s at different

columns.[18,19] The attempt is interesting but Strong [18] attributes orbitals by decreasing m_l values (Figure 2). For example, with transition elements, he assigns m_l equal 2 to column 3 then 1 to column 4 and so on decreasing up to -2 to column 7. A second series begins with m_l equal 2 in column 8 and ends with -2 in the column 12. However, the order changes slightly for lanthanides and actinides starting with m_l equal 2 instead of 3 (Figure 2). Stowe [19] did another choice by decreasing m_l from ℓ to $-\ell$ then he

changed the ranging from $-\ell$ to ℓ . Our proposition is different because we search a relationship of maximizing the descriptor values. We must start with the smallest value of m . In addition, because m_ℓ appears as an imaginary quantity in the expression of exact hydrogen atom orbitals, it would be wise to use only its absolute value.

So to differentiate orbitals of the same sub-shell, we propose to add a third contribution versus $|m_\ell|$ with weighting coefficient a_3 . For example, in the sub-shell 3d,

orbitals will be ranked in the following order: $|m_\ell| = 0, 1, 1, 2, 2, 0, 1, 1, 2, 2$ as it is shown in Figure 2. By this procedure, the 10 chemical elements of the sub-shell $(n-1)d$ will be separated on 3 groups associated with values of $|m_\ell|$ equal 0, 1 and 2. However, this addition has to not change the order of filling sub-shells. We propose for the weighting coefficient a_3 the value 0.0075 so that for the greatest $|m_\ell|$ value of $(n-2)f$ sub-shell, the contribution is equal to $3 * 0.0075 = 0.0225$. It remains below 0.75 which is the value between two successive sub-shells.

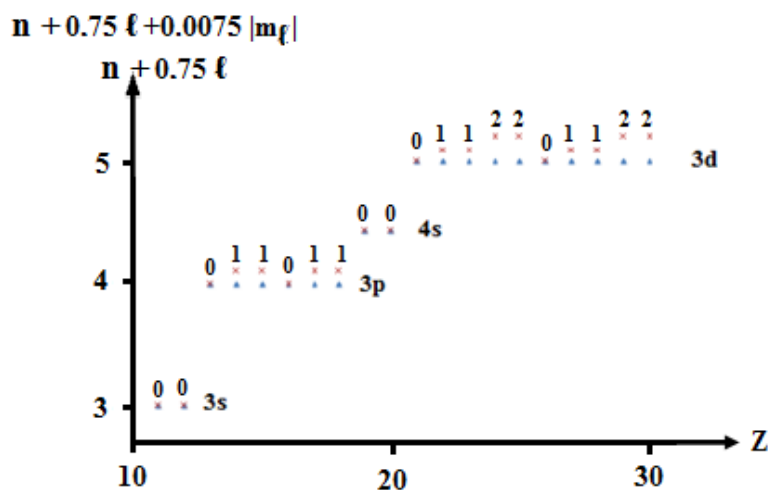


Figure 3. Visualization of the partial removing degeneration of the sub-shell orbitals. On bottom, we have the values of $(n+0.75\ell)$ and above those of $(n+0.75\ell + 0.0075|m_\ell|)$

Hund's rule also includes the spin quantum number m_s . Strong [18] attributes the value $+\frac{1}{2}$ to the first half of the sub-shell elements and $-\frac{1}{2}$ the second moiety (Figure 2).

Forcing the configuration to maximize its spin multiplicity is in favor of the intervention of S ($S = \sup(M_s)$ and $M_s = \sum_k m_{s_k}$). As the sub-shell is filled by electrons, $2 * S$ will increase to its maximum value equal to the number of orbitals of the sub-shell then decrease by steps of one until his minimum value of zero. We then add a weighting coefficient a_4 of 0.005 to reflect this contribution. So we still get a partial degeneration lift as we show in Table 1 for 3d sub-shell which $(n+\ell)$ is equal to 5. We will have different values between 4.7 and 4.9. They converse according $|m_\ell|$ in three groups associated with the values 0,

1 and 2. We see for example, that for each of the four items of value $|m_\ell| = 1$, the spin quantum number input is evaluated by various $0.005 * S$ with $2 * S$ denoting the number of single electrons that are 2 and 3 and 3 and 2 respectively.

The entire procedure we have just applied is based on the concept of the most recently added electron (MRA). It does not lead to a monotonically increasing trend because the evolution of $|m_\ell|$ a sub-shell is that of a sawtooth function and that of the spin quantum number is triangular. However, experimental electronic configuration of chromium or copper shows that the electronic configuration is in fact governed by the stability of the entire valence electrons. That's why we add a fifth contribution equal to the total number of occupied spinorbitales noted So .

Table 1. Values of non optimized five contributions intervening in the filling generalized formula for this work as well as the optimized value of the descriptor K_i .

Z	$n+\ell$	$a_1n+a_2\ell$	$a_1n+a_2+a_3 m_\ell $	$a_1n+a_2\ell + a_3 m_\ell +a_4S$	$a_1n+a_2\ell + a_3 m_\ell +a_4S+a_5So$	K_i
21	5	4.72	4.72	4.73	4.75	4,70
22	5	4.72	4.80	4.80	4.85	4,73
23	5	4.72	4.80	4.81	4.88	4,76
24	5	4.72	4.87	4.88	4.98	4,80
25	5	4.72	4.87	4.89	5.01	4,83
26	5	4.72	4.72	4.73	4.88	4,83
27	5	4.72	4.80	4.81	4.98	4,86
28	5	4.72	4.80	4.81	5.00	4,89
29	5	4.72	4.87	4.88	5.10	4,92
30	5	4.72	4.87	4.87	5.12	4,94

As it is necessary to compensate the behavior of $|m_\ell|$ and S that are not monotone increasing, we will choose a higher weighting coefficient a_5 equal to 0.025. Thus the maximum contribution associated with spinorbitals is $14 * 0.025 = 0.35$ remains below the coefficient 0.75 on the quantum number ℓ contribution.

We will therefore propose a formula which generalizes that used to this day, the Madelung-Klechkowski rule. It consists of calculating a real number noted K_i for the i th electron occupying a spinorbital whose expression is given by equation (3):

$$K_i = a_1 n + a_2 \ell + a_3 |m_\ell| + a_4 S + a_5 \quad (3)$$

We can also define a similar quantity for the atomic configuration, denoted $K(zX)$, by summing the N different values of K_i :

$$K(zX) = \sum_{i=1}^N K_i.$$

We have sought to optimize the values of the parameters a_k so as to obtain a monotonic evolution of K_i and $K(zX)$ as the atomic number Z increases. We obtained the following values by means of the simplex solver:

$$\begin{aligned} a_1 &= 1.07432 & a_2 &= 0.72374 & a_3 &= 0.00753 \\ a_4 &= 0.00575 & a_5 &= 0.02545. \end{aligned}$$

For easier use, we will only more simplified numbers:

$$\begin{aligned} a_1 &= 1.07 & a_2 &= 0.72 & a_3 &= 0.0075 \\ a_4 &= 0.0057 & a_5 &= 0.025. \end{aligned}$$

Table 2 indicates the calculation details for the two first rows of the standard periodic table.

Table 2. Details of the two first rows of the standard periodic table calculation of K_i and $K(zX)$

X	n	l	m	2S	So	K_i	$K(X)$
H	1	0	0	1	1	1.10	1.10
He	1	0	0	0	2	1.12	2.22
Li	2	0	0	1	1	2.17	4.39
Be	2	0	0	0	2	2.19	6.58
B	2	1	1	1	1	2.90	9.48
C	2	1	1	2	2	2.93	12.41
N	2	1	0	3	3	2.95	15.36
O	2	1	1	2	4	2.98	18.34
F	2	1	1	1	5	3.00	21.34
Ne	2	1	0	0	6	3.01	24.35

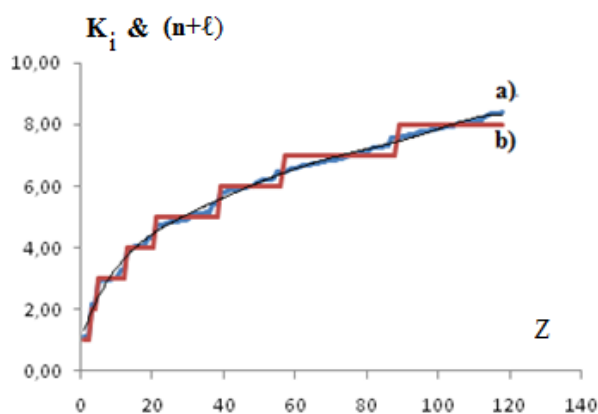


Figure 4. a) K_i and b) $(n+l)$ versus the atomic number Z

We present in the supplementary materials the calculations details of all chemical elements in the configuration expected by Madelung-Klechkowski rule. In order to compare our results to those obtained by the latter rule, we reported in Figure 4 K_i and $(n+l)$ values versus the atomic number Z .

It becomes clear that the Madelung-Klechkowski rule is a simplified way to describe the filling process of orbitals. Our proposed formula fits roughly with the following expression K_i versus Z :

$$K_i = -0.013Z^2 + 0.335Z + 0.994 \quad (R^2 = 0.99).$$

Figure 5 depicts the dependence of $K(zX)$ on Z . We obtain a very good parabolic correlation as:

$$K(zX) = 0.021Z^2 + 3.748Z - 15.90 \quad (R^2 = 0.99).$$

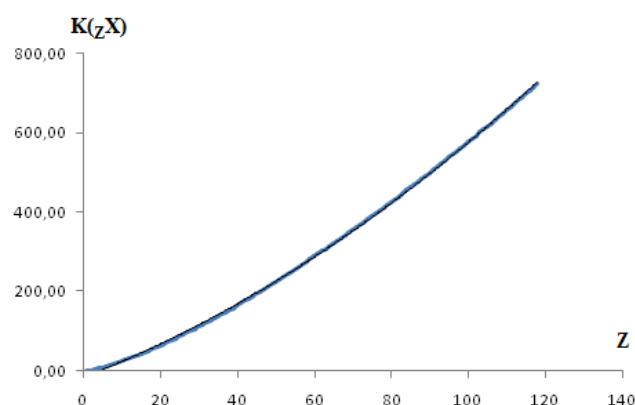


Figure 5. The variations of $K(zX)$ versus Z

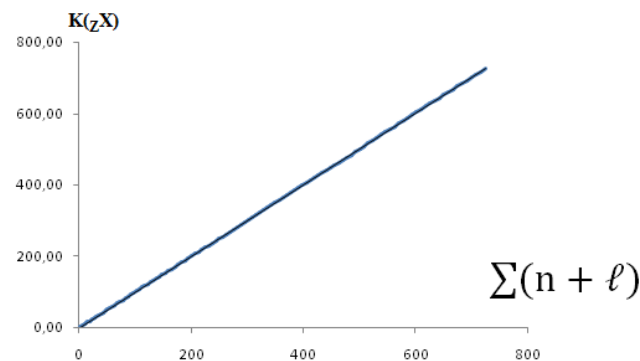


Figure 6. Variations of $K(zX)$ versus $\sum(n+l)$ values

From Figure 4, we can observe that $(n+l)$ values split each part of K_i roughly in its middle. For a fixed value of $(n+l)$, when Z increases, K_i is lower than it for the first chemical elements and higher for the other. So we obtain a linear correlation between $K(zX)$ and the $\sum(n+l)$ values as it is shown in Figure 6.

$$K(zX) = 1.004(n+l) - 1.267 \quad (R^2 = 1).$$

Since the proposed formulation incorporates several factors contributing to the stability of the atom in its ground state configuration, we tried to link the value of $K(zX)$ to the potential of first ionization $EI1(zX)$.

The challenge is a priori unrealizable because $K(zX)$ is an increasing function but $EI1$ is periodic in type. However this periodicity shows that the first value, the alkali one, is low. For the other values, changing $EI1$ is

almost linear. For that, we will treat each period separately by calculating $\Delta K(zX)$, the difference between $K(zX)$ and the value of the noble gas in the previous period.

$$\Delta K(zX) = K(zX) - K(zX_{GR}).$$

We will limit our work to blocks s and p that better generates the notion of periodicity than the nd and nf sub-shells.

We suppose that $\Delta K(zX)_I$ is proportional to EI1:

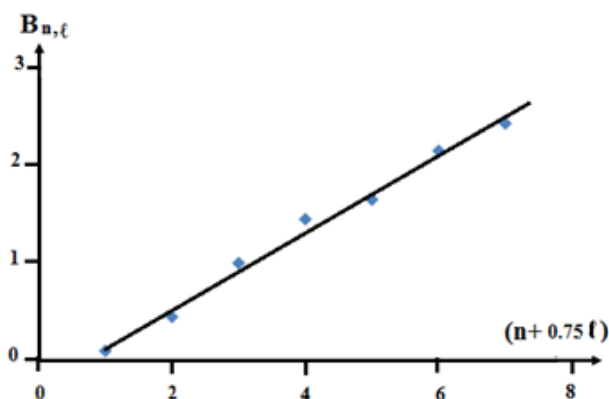
$$\Delta K(zX)_{n,\ell} = B_{n,\ell} EI1(zX)$$

Table 3. Optimized values of coefficients $B_{n,\ell}$ obtained by simplex solver

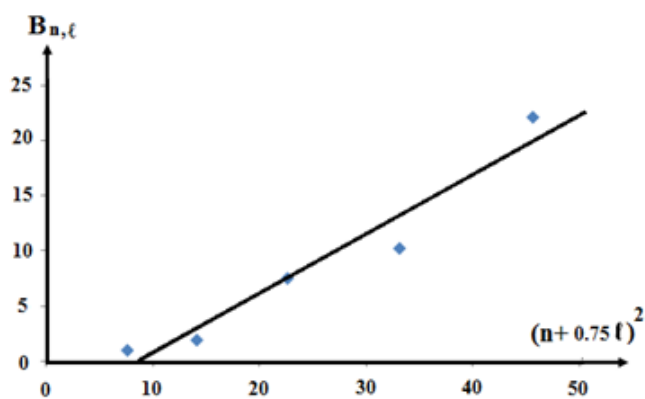
Sub-shell	$B_{n,\ell}$	value
1s	$B_{1,0}$	0.09
2s	$B_{2,0}$	0.44
2p	$B_{2,1}$	1.01
3s	$B_{3,0}$	0.99
3p	$B_{3,1}$	1.94
4s	$B_{4,0}$	1.44
4p	$B_{4,1}$	7.55
5s	$B_{5,0}$	1.64
5p	$B_{5,1}$	10.27
6s	$B_{6,0}$	2.14
6p	$A_{6,1}$	22.18
7s	$A_{7,0}$	2.42

where B_i is a coefficient to optimize so that the sum of $\frac{\Delta K(zX)_{n,\ell}}{B_{n,\ell}}$ is equal to the sum of experimental EI1 (zX) of each sub-shell:

$$\sum_k \frac{\Delta K(zX_k)_{n,\ell}}{B_{n,\ell}} = \sum_k EI1_k$$



(a)



(b)

Figure 8.

3. Conclusion

In this work, we established an empirical formula of a descriptor $K(zX)$ which generalizes the Madelung-Klechkowski rule. It is obtained by taking into account all

where k represents the index relative to an atom of the sub-shell. Table 3 contains the optimized values of coefficients $B_{n,\ell}$ obtained by simplex solver.

Figure 7 depicts the values of the first ionization energies and those obtained from our treatment based on the values of $K(zX)$. We can conclude that our method leads to approximate values of the first ionization energies of the major studied elements.

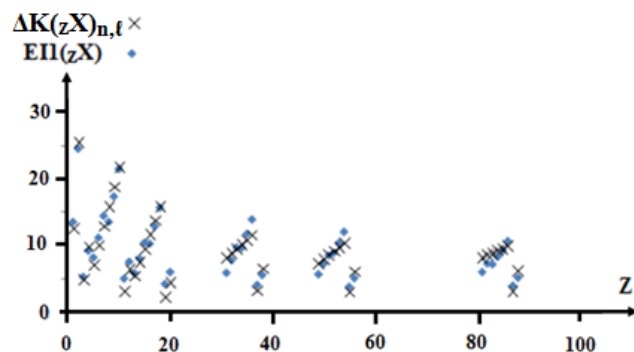


Figure 7. $\Delta K(zX)_{n,\ell}$ and $EI1(zX)$ versus the atomic number Z

We can find a correlation relationship (Figure 8) between the $B_{n,\ell}$ coefficients for each type of sub-shell according to the value $(n+0.75\ell)$. For the sub-shells ns, we find the linear relation:

$$B_{n,\ell} = 0.394(n + 0.75\ell) - 0.268 \quad (R^2 = 0.990).$$

For the sub-shells np, the linear relationship based on the value $(n + 0.75\ell)^2$ is:

$$B_{n,\ell} = 0.546(n + 0.75\ell)^2 - 4.821 \quad (R^2 = 0.941).$$

We can now propose the approximate expression of $B_{n,\ell}$:

$$B_{n,\ell} = (n + 0.75\ell)^{\ell+1}.$$

the electrons from the atom to describe the ground state electronic configuration. $K(zX)$ is a good descriptor of the atom stability because it is directly related to the ionization potential. It is so intuitive to expect that $K(zX)$ would be able to lead to the exact configuration of all the chemical elements and to overcome all exceptions. Work is in progress concerning the exceptions.

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Supplementary Material

Calculation details of K_i and $K(zX)$ for all chemical elements

X	Z	CONFIGURATION	n	l	m	2*S	So	K_i	n+l	$K(X)$	$\Sigma(n+l)$
H	1	1s ¹	1	0	0	1	1	1.10	1	1,10	1
He	2	1s ²	1	0	0	0	2	1.12	1	2,23	2
Li	3	[He]2s ¹	2	0	0	1	0	2.17	2	4,38	4
Be	4	[He]2s ²	2	0	0	0	2	2.19	2	6,58	6
B	5	[He]2s ² 2p ¹	2	1	0	1	1	2.90	3	9,48	9
C	6	[He]2s ² 2p ²	2	1	1	2	2	2.93	3	12,42	12
N	7	[He]2s ² 2p ³	2	1	1	3	3	2.95	3	15,38	15
O	8	[He]2s ² 2p ⁴	2	1	0	2	4	2.98	3	18,36	18
F	9	[He]2s ² 2p ⁵	2	1	1	1	5	3.00	3	21,37	21
Ne	10	[He]2s ² 2p ⁶	2	1	1	0	6	3.01	3	24,40	24
Na	11	[Ne]3s ¹	3	0	0	1	1	3,25	3	27,65	27
Mg	12	[Ne]3s ²	3	0	0	0	2	3,27	3	30,93	30
Al	13	[Ne]3s ² 2p ¹	3	1	0	1	1	3,98	4	34,90	34
Si	14	[Ne]3s ² 2p ²	3	1	1	2	2	4,01	4	38,91	38
P	15	[Ne]3s ² 2p ³	3	1	1	3	3	4,04	4	42,95	42
S	16	[Ne]3s ² 2p ⁴	3	1	0	2	4	4,05	4	47,01	46
Cl	17	[Ne]3s ² 2p ⁵	3	1	1	1	5	4,08	4	51,09	50
Ar	18	[Ne]3s ² 2p ⁶	3	1	1	0	6	4,11	4	55,20	54
K	19	[Ar]4s ¹	4	0	0	1	1	4,33	4	59,53	58
Ca	20	[Ar]4s ²	4	0	0	0	2	4,35	4	63,87	62
Sc	21	[Ar]4s ² 3d ¹	3	2	0	1	1	4,70	5	68,57	67
Ti	22	[Ar]4s ² 3d ²	3	2	1	2	2	4,73	5	73,31	72
V	23	[Ar]4s ² 3d ³	3	2	1	3	3	4,76	5	78,07	77
Cr	24	[Ar]4s ¹ 3d ⁵	3	2	2	4	4	4,80	5	82,87	82
Mn	25	[Ar]4s ² 3d ⁵	3	2	2	5	5	4,83	5	87,70	87
Fe	26	[Ar]4s ² 3d ⁶	3	2	0	4	6	4,83	5	92,53	92
Co	27	[Ar]4s ² 3d ⁷	3	2	1	3	7	4,86	5	97,39	97
Ni	28	[Ar]4s ² 3d ⁸	3	2	1	2	8	4,89	5	102,28	102
Cu	29	[Ar]4s ¹ 3d ¹⁰	3	2	2	1	9	4,92	5	107,20	107
Zn	30	[Ar]4s ² 3d ¹⁰	3	2	2	0	10	4,94	5	112,14	112
Ga	31	[Ar]4s ² 3d ¹⁰ 4p ¹	4	1	0	1	1	5,05	5	117,19	117
Ge	32	[Ar]4s ² 3d ¹⁰ 4p ²	4	1	1	2	2	5,09	5	122,27	122
As	33	[Ar]4s ² 3d ¹⁰ 4p ³	4	1	1	3	3	5,11	5	127,39	127
Se	34	[Ar]4s ² 3d ¹⁰ 4p ⁴	4	1	0	2	4	5,13	5	132,52	132

X	Z	CONFIGURATION	n	ℓ	m	2*S	So	K _i	n+ℓ	K(X)	Σ(n+ℓ)
Br	35	[Ar]4s ² 3d ¹⁰ 4p ⁵	4	1	1	1	5	5,16	5	137,68	137
Kr	36	[Ar]4s ² 3d ¹⁰ 4p ⁶	4	1	1	0	6	5,18	5	142,86	142
Rb	37	[Kr]5s ¹	5	0	0	1	1	5,40	5	148,26	147
Sr	38	[Kr]5s ²	5	0	0	0	2	5,42	5	153,68	152
Y	39	[Kr]5s ² 4d ¹	4	2	0	1	1	5,77	6	159,45	158
Zr	40	[Kr]5s ² 4d ²	4	2	1	2	2	5,81	6	165,26	164
Nb	41	[Kr]5s ¹ 4d ⁴	4	2	1	3	3	5,84	6	171,10	170
Mo	42	[Kr]5s ¹ 4d ⁵	4	2	2	4	4	5,87	6	176,97	176
Tc	43	[Kr]5s ¹ 4d ⁶	4	2	2	5	5	5,90	6	182,87	182
Ru	44	[Kr]5s ¹ 4d ⁷	4	2	0	4	6	5,91	6	188,78	188
Rh	45	[Kr]5s ¹ 4d ⁸	4	2	1	3	7	5,94	6	194,72	194
Pd	46	[Kr]5s ⁰ 4d ¹⁰	4	2	1	2	8	5,96	6	200,68	200
Ag	47	[Kr]5s ¹ 4d ¹⁰	4	2	2	1	9	5,99	6	206,67	206
Cd	48	[Kr]5s ² 4d ¹⁰	4	2	2	0	10	6,01	6	212,69	212
In	49	[Kr]5s ² 4d ¹⁰ 5p ¹	5	1	0	1	1	6,12	6	218,81	218
Sn	50	[Kr]5s ² 4d ¹⁰ 5p ²	5	1	1	2	2	6,16	6	224,97	224
Sb	51	[Kr]5s ² 4d ¹⁰ 5p ³	5	1	1	3	3	6,19	6	231,16	230
Te	52	[Kr]5s ² 4d ¹⁰ 5p ⁴	5	1	0	2	4	6,20	6	237,36	236
I	53	[Kr]5s ² 4d ¹⁰ 5p ⁵	5	1	1	1	5	6,23	6	243,60	242
Xe	54	[Kr]5s ² 4d ¹⁰ 5p ⁶	5	1	1	0	6	6,26	6	249,85	248
Cs	55	[Xe]6s ¹	6	0	0	1	1	6,47	6	256,33	254
Ba	56	[Xe]6s ²	6	0	0	0	2	6,50	6	262,82	260
La	57	[Xe]6s ² 5d ¹	4	3	0	1	1	6,50	7	269,32	267
Ce	58	[Xe]6s ² 4f ²	4	3	1	2	2	6,53	7	275,85	274
Pr	59	[Xe]6s ² 4f ³	4	3	1	3	3	6,56	7	282,41	281
Nd	60	[Xe]6s ² 4f ⁴	4	3	2	4	4	6,60	7	289,01	288
Pm	61	[Xe]6s ² 4f ⁵	4	3	2	5	5	6,63	7	295,63	295
Sm	62	[Xe]6s ² 4f ⁶	4	3	3	6	6	6,66	7	302,30	302
Eu	63	[Xe]6s ² 4f ⁷	4	3	3	7	7	6,69	7	308,99	309
Gd	64	[Xe]6s ² 5d ¹ 4f ⁷	4	3	0	6	8	6,69	7	315,67	316
Tb	65	[Xe]6s ² 4f ⁹	4	3	1	5	9	6,72	7	322,39	323
Dy	66	[Xe]6s ² 4f ¹⁰	4	3	1	4	10	6,74	7	329,14	330
Ho	67	[Xe]6s ² 4f ¹¹	4	3	2	3	11	6,77	7	335,91	337
Er	68	[Xe]6s ² 4f ¹²	4	3	2	2	12	6,79	7	342,70	344
Tm	69	[Xe]6s ² 4f ¹³	4	3	3	1	13	6,82	7	349,53	351
Yb	70	[Xe]6s ² 4f ¹⁴	4	3	3	0	14	6,85	7	356,38	358
Lu	71	[Xe]6s ² 4f ¹⁴ 5d ¹	5	2	0	1	1	6,85	7	363,22	365
Hf	72	[Xe]6s ² 4f ¹⁴ 5d ²	5	2	1	2	2	6,88	7	370,11	372
Ta	73	[Xe]6s ² 4f ¹⁴ 5d ³	5	2	1	3	3	6,91	7	377,02	379
W	74	[Xe]6s ² 4f ¹⁴ 5d ⁴	5	2	2	4	4	6,95	7	383,96	386
Re	75	[Xe]6s ² 4f ¹⁴ 5d ⁵	5	2	2	5	5	6,98	7	390,94	393
Os	76	[Xe]6s ² 4f ¹⁴ 5d ⁶	5	2	0	4	6	6,98	7	397,92	400
Ir	77	[Xe]6s ² 4f ¹⁴ 5d ⁷	5	2	1	3	7	7,01	7	404,94	407
Pt	78	[Xe]6s ¹ 4f ¹⁴ 5d ⁹	5	2	1	2	8	7,04	7	411,97	414
Au	79	[Xe]6s ¹ 4f ¹⁴ 5d ¹⁰	5	2	2	1	9	7,07	7	419,04	421
Hg	80	[Xe]6s ² 4f ¹⁴ 5d ¹⁰	5	2	2	0	10	7,09	7	426,13	428
Tl	81	[Xe]6s ² 4f ¹⁴ 5d ¹⁰ 5p ¹	6	1	0	1	1	7,20	7	433,33	435
Pb	82	[Xe]6s ² 4f ¹⁴ 5d ¹⁰ 5p ²	6	1	1	2	2	7,23	7	440,56	442
Bi	83	[Xe]6s ² 4f ¹⁴ 5d ¹⁰ 5p ³	6	1	1	3	3	7,26	7	447,82	449
Po	84	[Xe]6s ² 4f ¹⁴ 5d ¹⁰ 5p ⁴	6	1	0	2	4	7,28	7	455,10	456
At	85	[Xe]6s ² 4f ¹⁴ 5d ¹⁰ 5p ⁵	6	1	1	1	5	7,31	7	462,41	463

X	Z	CONFIGURATION	n	ℓ	m	2*S	So	K _i	n+ℓ	K(X)	Σ(n+ℓ)
Rn	86	[Xe]6s ² 4f ¹⁴ 5d ¹⁰ 5p ⁶	6	1	1	0	6	7,33	7	469,74	470
Fr	87	[Re]7s ¹	7	0	0	1	1	7,55	7	477,28	477
Ra	88	[Re]7s ²	7	0	0	0	2	7,57	7	484,86	484
Ac	89	[Re]7s ² 6d ¹	5	3	0	1	1	7,57	8	492,43	492
Th	90	[Re]7s ² 6d ²	5	3	1	2	2	7,61	8	500,03	500
Pa	91	[Re]7s ² 6d ¹ 5f ²	5	3	1	3	3	7,64	8	507,67	508
U	92	[Re]7s ² 6d ¹ 5f ³	5	3	2	4	4	7,67	8	515,34	516
Np	93	[Re]7s ² 6d ⁰ 5f ⁵	5	3	2	5	5	7,70	8	523,04	524
Pu	94	[Re]7s ² 6d ⁰ 5f ⁶	5	3	3	6	6	7,74	8	530,78	532
Am	95	[Re]7s ² 6d ⁰ 5f ⁷	5	3	3	7	7	7,76	8	538,54	540
Cm	96	[Re]7s ² 6d ¹ 5f ⁷	5	3	0	6	8	7,76	8	546,30	548
Bk	97	[Re]7s ² 6d ¹ 5f ⁸	5	3	1	5	9	7,79	8	554,10	556
Cf	98	[Re]7s ² 6d ⁰ 5f ¹⁰	5	3	1	4	10	7,82	8	561,91	564
Es	99	[Re]7s ² 6d ⁰ 5f ¹¹	5	3	2	3	11	7,85	8	569,76	572
Fm	100	[Re]7s ² 6d ⁰ 5f ¹²	5	3	2	2	12	7,87	8	577,63	580
Md	101	[Re]7s ² 6d ⁰ 5f ¹³	5	3	3	1	13	7,90	8	585,53	588
No	102	[Re]7s ² 6d ⁰ 5f ¹⁴	5	3	3	0	14	7,92	8	593,45	596
Lr	103	[Re]7s ² 4f ¹⁴ 6d ¹	6	2	0	1	1	7,92	8	601,37	604
Rf	104	[Re]7s ² 4f ¹⁴ 6d ²	6	2	1	2	2	7,96	8	609,33	612
Db	105	[Re]7s ² 4f ¹⁴ 6d ³	6	2	1	3	3	7,99	8	617,31	620
Sg	106	[Re]7s ² 4f ¹⁴ 6d ⁴	6	2	2	4	4	8,02	8	625,34	628
Bh	107	[Re]7s ² 4f ¹⁴ 6d ⁵	6	2	2	5	5	8,05	8	633,39	636
Hs	108	[Re]7s ² 4f ¹⁴ 6d ⁶	6	2	0	4	6	8,06	8	641,44	644
Mt	109	[Re]7s ² 4f ¹⁴ 6d ⁷	6	2	1	3	7	8,09	8	649,53	652
Ds	110	[Re]7s ¹ 4f ¹⁴ 6d ⁹	6	2	1	2	8	8,11	8	657,64	660
Rg	111	[Re]7s ¹ 4f ¹⁴ 6d ¹⁰	6	2	2	1	9	8,14	8	665,78	668
Cn	112	[Re]7s ² 4f ¹⁴ 6d ¹⁰	6	2	2	0	10	8,16	8	673,95	676
Uut	113	[Re]7s ² 4f ¹⁴ 6d ¹⁰ 7p ¹	7	1	0	1	1	8,27	8	682,22	684
Fl	114	[Re]7s ² 4f ¹⁴ 6d ¹⁰ 7p ²	7	1	1	2	2	8,31	8	690,53	692
Uup	115	[Re]7s ² 4f ¹⁴ 6d ¹⁰ 7p ³	7	1	1	3	3	8,34	8	698,86	700
Lv	116	[Re]7s ² 4f ¹⁴ 6d ¹⁰ 7p ⁴	7	1	0	2	4	8,35	8	707,21	708
Uus	117	[Re]7s ² 4f ¹⁴ 6d ¹⁰ 7p ⁵	7	1	1	1	5	8,38	8	715,60	716
Uuo	118	[Re]7s ² 4f ¹⁴ 6d ¹⁰ 7p ⁶	7	1	1	0	6	8,40	8	724,00	724