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Interpretation of Some Atomistic Concepts from the Characteristic Graph of the Atom

Ousmane Barry, Mamadou Yaya Balde, Souleymane Balde*, Aboubacar Safie Sylla

Department of Chemistry, University Gamal Abdel Nasser of Conakry, Conakry, Guinea
Email: ousmanedounet@gmail.com, safiesylla9@gmail.com, baldez201073@gmail.com, *souleybal2@gmail.com

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Abstract

The study of the characteristic graph of an atom in all its aspects, allows to describe the concepts of atomistic. From this graph, some concepts of the recomposition of the electronic cloud have been described by specific graphs derived from it. The results are very conclusive. This graph illustrates each of the concepts of atomistics such as blocks, orders, periods and electronic layers. These concepts have been represented by lines, segments and even points. This has made it possible to draw up tables with orders, periods and even their correlations. Thus, this work promotes a better understanding of theoretical concepts by transposing the "abstract" aspect to a more "concrete" aspect of these concepts. This eventually facilitates the learning of this essential part of chemistry at its core. These results indicate that the research hypothesis has been verified.

Keywords

Electronic Cloud, Order, Period, Layers, Blocks

1. Introduction

From the antiquity to the current classification, the study of the atom is characterized by the succession of several theories. At the beginning of the 19th century, these theories were supported by experimentations. Today, many interesting and well-founded principles, laws and rules have been developed to better understand the phenomena of study [1].

In spite of these experiments, the rules and principles that are formulated convey a rather abstract character. These reasons continue to give rise to concerns and serious problems in understanding the formidable field of chemistry that is atomistics.

On the other hand, the evolution of conceptions on the structure of the atom has undergone several milestones. The knowledge of the atom beyond its literary meaning developed with the discovery of its smaller particles (electrons, protons, neutrons). The evolution of such a development is reflected in a fairly coherent timeline [2].

In 1808 John Dalton demonstrated that matter is made up of atoms, particles that are indivisible but different depending on the nature of the matter. A few decades later, in 1897 Thomson proved experimentally the existence of the electron in the laboratory. He formulated the hypothesis that the atom is the sum of positive and negative charges which are united in a homogeneous way. Subsequently, in 1911 Rutherford demonstrated the lacunar structure of atoms and indicated that the positive particles are concentrated in very small volumes forming nuclei and that the electrons gravitate around them at different energy levels. In 1913 Niels Bohr, using the quantum method (atomic spectroscopy), demonstrated that the energy of an electron is quantified, hence the main quantum number "n". He establishes that the trajectory of the electron is carried out on stationary orbits around the nucleus; on these orbits the energy of the electron is invariable; these orbits are today the electronic layers. A few years later, in 1917 Arnold Sommerfeld improved Bohr's method. He indicated that the movement of the electron is elliptical; this implies the secondary and magnetic quantum number, characteristic of the atomic orbitals. He affirms that the electron is different from a material point.

In 1924 Louis De Broglie associated a wave with any particle in motion, especially when it is infinitesimal. After one year Werner Heisenberg stated the uncertainty principle on the simultaneous very precise knowledge of the position and the speed of a particle such as the electron. In the same year, 1925, Erwin Schrödinger described the movement of the electron by a wave equation that bears his name; hence wave mechanics. He explains that the electrons around the nucleus are on atomic orbitals, *i.e.* the sublayers (s, p, d, f). He thus introduced the notion of the electron cloud, which is still valid today [2].

The atom is a particle structured in two (2) distinct fundamental regions according to Rutherford [2]. The nucleus is made up of nucleons (protons and neutrons) occupying the same position in the atom and forming a single population of the same energy level, *i.e.* a degenerate population. It is the seat of a very intense repulsion force; this force is the basis of the fission reaction limiting the number of natural atoms in general. This is at the threshold of 100, with artificial atoms the known number of atoms is 118 [3]. The electron cloud is the space in which the electrons move. Unlike nucleons, electrons are totally different from each other in the same atom by the energy levels they occupy. The different solutions of the Schrödinger equation are the main characteristics of electrons. Today, the electrons of an atom are defined by a quantum set (n, l, m, s). The first three parameters are the solutions of the Schrödinger equation, the fourth characterizes the rotation of the electron on itself. The interdependence of the first three quantum numbers defines all the forms of energy that differentiate the electrons of an atom. The electrons that are supposed to be closest to each other differ by the fourth parameter. An atom can never have two identical electrons, even the heaviest (118 electrons); they are all individually different. This fact divides them into different populations, each with its own energy level, hence the Pauli exclusion principle [4]. Knowledge of the structure of the electron cloud consists of identifying the different energy levels that can explain the position of each electron in an atom in its ground state. Therefore, the structure of an atom in its ground state poses a real problem for identifying the different energy levels that make up the electron cloud.

The establishment of these energy levels is done through literary diagrams which are, among others: the Klechkowski rule, the spaghetti rule, the poly-electronic atom energy diagram, the 49-square checkerboard model, the Russian model. All of these characterizse the principle of filling the energy level of the orbitals [5]. These different schemes are still complex enough to be memorized logically or simply. The multiplicity of these proposed literary diagrams even intensifies the difficulty of understanding the classification, making it more difficult to memorize the positioning of the 22 "elements", *i.e.* the sub-layers of the electron cloud divided into four (4) blocks, including 7 "elements" for the "s" block (1s-7s), 6 "elements" for the "p" block (2p-7p), 5 "elements" for the "d" block (3d-7d) and, finally, 4 others for the "f" block (4f-7f).

To work out the order of positioning of the elements of the electron cloud, principles and/or rules have been developed and refined over time. In 1936 Ervin Madelung developed the rule for the order of filling the different atomic orbitals. Subsequently, in 1962 Vsevolod Mavrikievih Klechkowski justified for the first time and generalised the importance of this energy level order given by the formula $O_E = n + l$, hence the rule that bears his name [6].

In sum, the whole atomistic theory conveys enough concepts that remain sufficiently abstract. The atom itself is an infinitesimal particle; to speak of others within it is even more minute and of course abstract, mainly at the level of young users (pupils, students and teachers). So many concerns that serve as a reference to promote the search for new, more concrete scientific models, *i.e.* to innovate with new, more or less consumable proposals in this rather abstract field of atomistics.

This work is a continuation of a publication in the Journal of Applied Mathematics and Physics (JAMP) [7]. It deals with the explanation of the concepts of atomistics by the elements of analytic geometry, accessing very elementary notions such as "the point" and/or "the line". The characteristic graph of the atom [7] [8], which correlates all the literary diagrams, explains the composition of the electron cloud by points and lines representing each concept of atomistics; they are easily spotted and logically interpretable and are prepared to be known and memorized as simply as possible. They express the most important facts of atomistics.

The aim of this work is to develop creative imaginations instead of the classical methods, which are ambiguous because of their rather abstract character.

Obtaining the specific graphs from the characteristic graph of the atom has been explained in the methodology part. Electronic cloud concepts were illustrated and discussed and a conclusion was made.

2. Methods

The characteristic graph of the atom is constructed in an orthonormal axis system of the type (n, N, O_E): a plane whose origin is the nucleus "N", the abscissa is the period "n" and the ordinate is the energy level order "O_E". In this graph, the sub-layers are the different points of the plane. The grouping of these into layer, block, period and order is presented in the form of straight lines.

A point is the intersection of several lines; a line is an infinite succession of points. The line can be a segment if it is limited at both ends, thus designating a definite concept; a half-line if it is limited at one end, designating an indefinite concept. The lines are horizontal, vertical, oblique and even broken; they are either parallel or intersecting. Each of these component lines of the atom's characteristic graph can represent a salient fact or concept in atomistics [7].

The use of the graph already elaborated and published [7] makes it possible to illustrate all the concepts of atomistics. The simplest way to draw it is to draw the system of orthonormal axes (n, N, O_E): the first and last sub-layer of each block are represented according to their coordinates (n, O_E). Then connect them by straight lines of equation:

$$O_E = n + \ell \tag{1}$$

In Figure 1, blocks 1s-7s, 2p-7p, 3d-7d and 4f-7f are represented by segments. This graph is completed by plotting horizontal lines (or asymptotes) of the type:

$$O_E = k \tag{2}$$

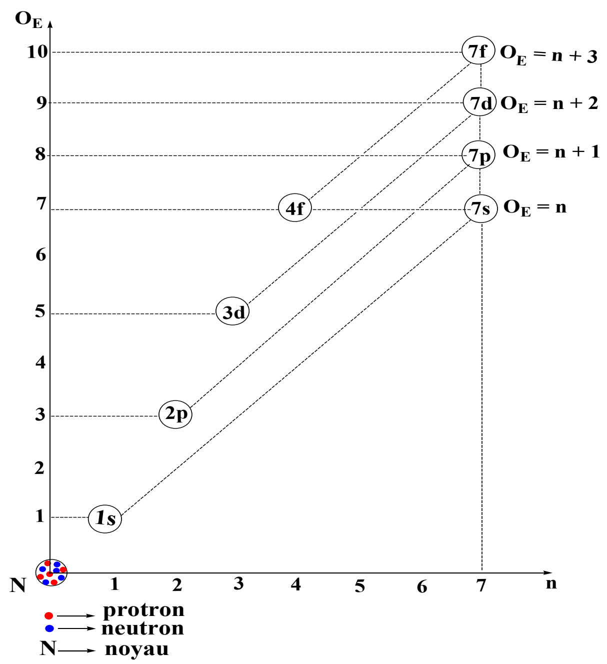


Figure 1. Representation of blocks by line segments.

with k ranging from 1 to 10; for k ranging from 1 to 7, these lines end on the segment of block "s", and the others end on the elements of layer 7. The graph also contains vertical lines (or asymptotes) of the type

$$n = k' \tag{3}$$

With k' ranging from 1 to 7; by analogy, these vertical asymptotes end on the "*f*" block when k' takes the values 4, 5, 6 and 7; for values of k' lower than 4, they end on the beginning of the "s", "p" and "d" blocks respectively for $k' = 1$, $k' = 2$ and $k' = 3$.

This thus results in **Figure 2** showing the arrangement of all the sub-shells of the electron cloud.

Figure 2 is the intersection of the various straight lines indicating the position of the intermediate sub-shells at each block, which form the electron cloud of the atom. **Figure 3**, characteristic of the atom, results by replacing the various points of intersection of the straight lines by the corresponding subshells. This is the illustration of the "new overview of the energy classification of sublayers" [7].

Such a graph can be obtained by representing each of the 22 subshells according to their coordinates (n; O_E) and by drawing these different lines. The elaboration of this graph simultaneously solves several problems related to the concepts of atomistics such as layers, blocks, periods, orders etc. Indeed, each of these concepts can be described by a specific graph and represented by points, segments, half-lines or lines.

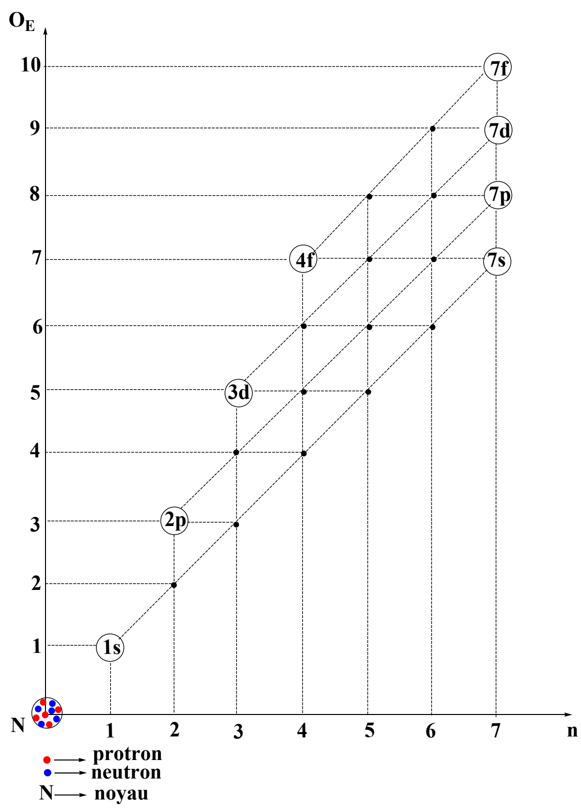


Figure 2. Positioning of the electronic cloud sublayers.

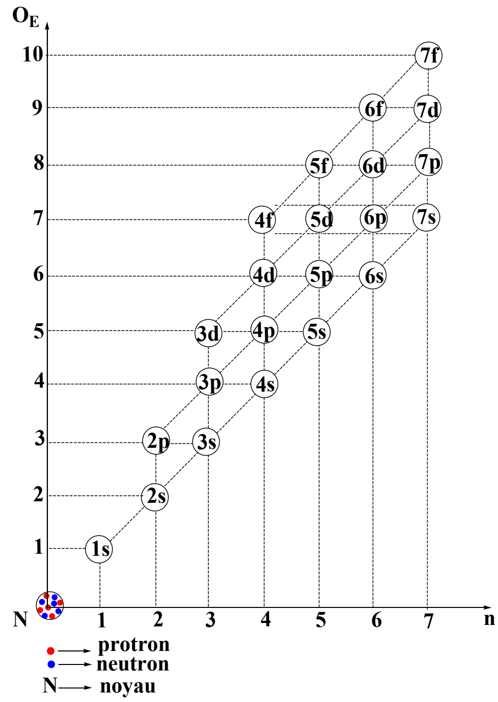


Figure 3. Characteristic of the atom.

3. Results

The developed graph (Figure 3) allows for more perfect illustrations of a set of concepts on atomistics. It promotes a better understanding of theoretical concepts by moving from the "abstract" to a more "concrete" aspect of these concepts. This eventually facilitates the learning of this essential part of chemistry at its core. An illustration of some concepts such as the different groupings of the electron cloud; *i.e.* electron layers, element blocks, order and period is presented by specific graphs.

3.1. Illustration of Electronic Layers

The layers are represented by the vertical asymptotes of type $n = k'$ (k ranging from 1 to 7). By masking the horizontal and oblique lines of the characteristic graph of the atom, the electronic cloud is recomposed into groups according to Figure 4.

3.2. Illustration of Blocks

By abandoning the horizontal and vertical lines of the characteristic graph of the atom, the electronic cloud is recomposed into a block represented by segments of equation $O_E = n + \ell$. The slope of each of the segments is:

$$a = \frac{O_{E2} - O_{E1}}{n_2 - n_1} = 1 \tag{4}$$

which aligns all sub-layers of the same nature in a block. The different blocks are parallel (properties of straight lines in geometry). The straight lines, representing the blocks, never cut the axes. This finding is explained by the fact that the electron never falls into the nucleus (Bohr's postulate). Academically, these lines would intersect the axes at their coordinates at the origin, which are respectively 0, 1, 2 and 3 at the different blocks (spdf). These coordinates at the origin are the respective secondary quantum numbers of these different subshells as shown in Figure 5.

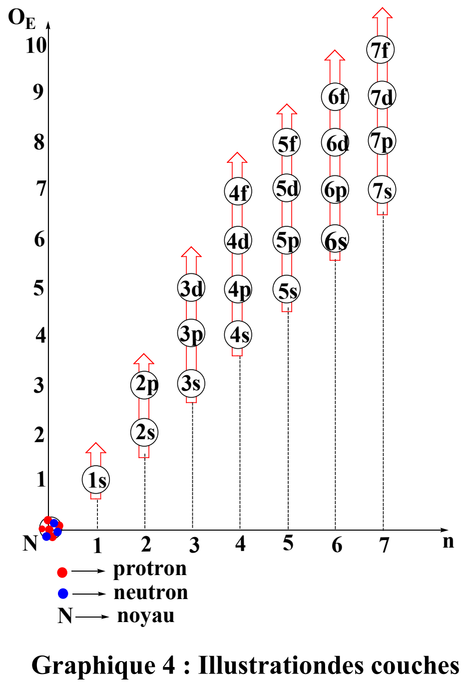


Figure 4. Ilustration of layers.

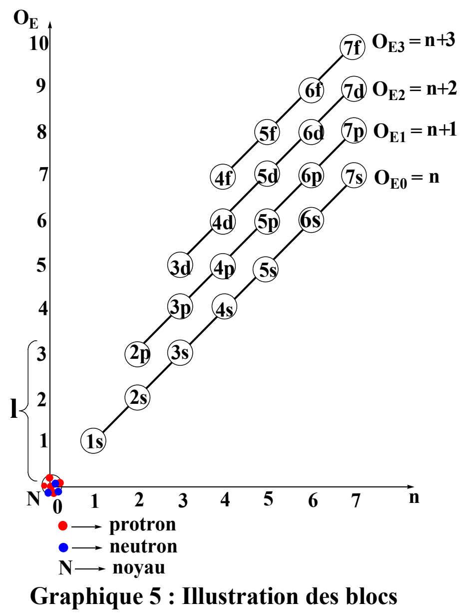


Figure 5. Ilustration of blocks.

3.3. Illustration of Orders

The illustration of the "orders" is carried out on the basis of **Figure 3**, keeping only the horizontal asymptotes $O_E = k$ with k ranging from 1 to 8 practically. Each value of k indicates the classification of the sub-layers of the same order according to the increasing "n" period; moreover, the number of sub-layers is a function of the size of the order. For example, for k equal to 1 and 2, the respective orders are formed by one sub-layer each (1s and 2s). If k equals 3 and 4, the orders are two sublayers (2p 3s and 3p 4s respectively). When k is 5 and 6, there are three sub-layers which are 3d 4p 5s, 4d 5p 6s respectively. The highest order is for k equal to 7 with four sub-layers which are: 4f 5d 6p 7s. For k equals 8, the order is undefined.

This shows that an order always ends with the sublayer "s" and can start with any sublayer depending on the size of the order. Thus, the structure of the "order" becomes quantifiable and is expressed by the relation:

$$(n-3)\text{f},\ (n-2)\text{d},\ (n-1)\text{p}\ \ n\text{s} \tag{5}$$

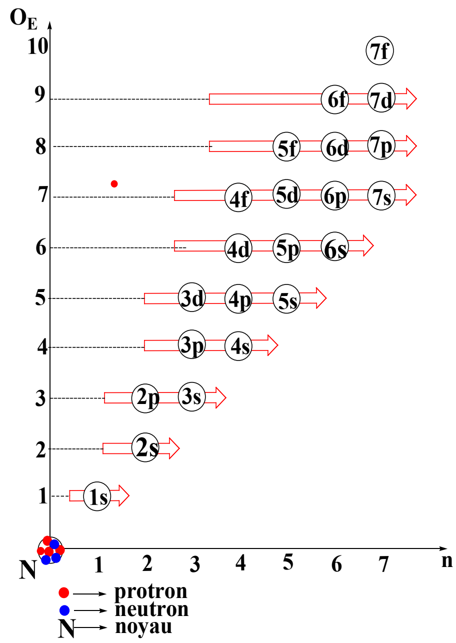
For the block "s": $O_E = n$. The order-specific graph developed in this way is an effective tool for better understanding the Klechkowski rule. **Figure 6** perfectly illustrates this rule and the principle of Aufbau (stacked construction).

3.4. Illutration of Periods

The periods are 8, 18 and 32 columns, *i.e.* short, medium and long. Here we present the long period graph. For this purpose, the segments representing the blocks shown in the figure characterizing the atom are removed. The periods, like the layers, are defined along the abscissa of the graph. A period is defined, for the most part, by the intersection between two successive orders and two or three consecutive layers except for $n = 1$ and 2, for which the electronic layer is identical to the period. However, even for $n = 2$, the layer or period lies between two orders. For $n \geq 3$, the periods become more complicated and lie on a quadrilateral or quadrilaterals resulting from the intersection between successive orders and consecutive layers. The period is thus a part of the elements of this quadrilateral going from the lower right vertex "ns" to the upper left vertex "(n – 1)d" and/or "(n – 2)f" of the transition elements and including all the elements of the upper side up to "np". Thus a period always starts with the sub-layer "ns" and ends with "np" and the intermediate sub-layers are necessarily transition elements "d" and "f" whose coefficients are (n – 1) for "d" and (n – 2) for "f". This observation thus makes it possible to define a coherent limit of the structure of a period according to the values admitted by the relation: "ns (n – 2)f (n – 1)d np".

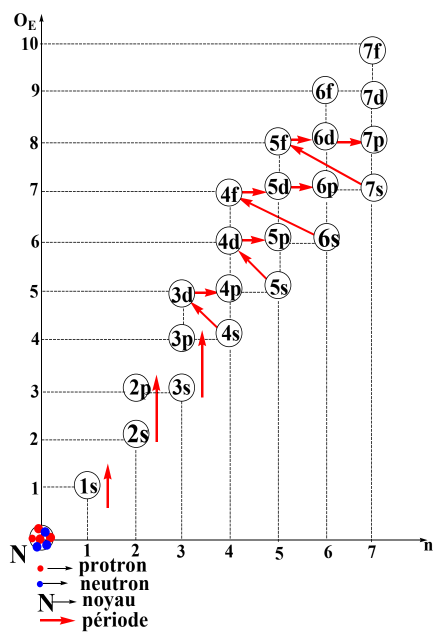
It should be noted that the sub-layers "s" and "p" have the same coefficients (period number). For example, for $n = 1$, the period is formed by a sub-layer "1s" according to the accepted values. However, if n is equal to 2 and 3, there are two sublayers per period: "2s 2p" and "3s 3p". For "n" ranging from 4 to 5, there are three sub-layers with the appearance of the first transition elements: "4s 3d 4p" and "5s 4d 5p". For the last two periods, there are four sub-layers with all transition elements: "6s 4f 5d 6p" and "7s 5f 6d 7p".

Order and period are subject to the principle of stability. Figure 7 depicts the difference between order and period.



Graphique 6 : Illustration des ordres

Figure 6. Ilustration of orders.



Graphique 7 : Illustration des périodes

Figure 7. Ilustration of periods.

Table 1. Group of subshells according to the order of energy [(n − 3)f (n − 2)d (n − 1)p ns].

Orders O_E	1	2	3	4	5	6	7	8
Sub-shells	1s	2s	2p 3s	3p 4s	3d 4p 5s	4d 5p 6s	4f 5d 6p 7s	5f 6d 7p…

Table 2. Group of subshells according to the period [ns (n − 2)f (n − 1)d np].

Period n	1	2	3	4	5	6	7
Underlays	1s	2s 2p	3s 3p	4s 3d 4p	5s 4d 5p	6s 4f 5d 6p	7s 5f 6d 7p

Table 3. Relationship between period and order.

Period	1	2		3		4		5		6		7	
Subshells	1s	2s	2p	3s	3p	4s	3d 4p	5s	4d 5p	6s	4f 5d 6p	7s	5f 6d 7p…
Order	1	2	3		4		5		6		7		8

4. Discussion

Figure 4 and Figure 5 are not subject to the stability rule, unlike Figure 6 and Figure 7, which describe the composition of the elements of the electron cloud in order (Figure 6) and in period (Figure 7). The arrangement of the sublayers from "1s" to "7p" is practically in the order of increasing energy level either by O_E or by n in the usual ordering of natural numbers.

The structure of an order according to the accepted values is (n − 3)f (n − 2)d (n − 1)p ns. That of the period is ns (n − 2)f (n − 1)d np. It is remarkable that the order ends with the sub-layer "ns", whereas it can start with any sub-layer, even "ns" if the order is short, for example, for n = 1 or 2. In practice, orders range from 1 to 8. For periods, they start with "ns" and end with "np". The coefficients of the intermediate sub-layers are counted from "n" up to the limit values or allowed values. The order is then different from the period which goes from 1 to 7. The coefficients of the sublayers in each case are related to O_E and/or n, where for the block "s" $O_E = n$.

Thus, it is sufficient to be able to count from 1 to 7 and/or from 1 to 8 to elaborate the stability rule. Table 1 and Table 2, derived from graphs 6 and 7, allow the classification of the 22 atomic orbitals according to their increasing energy order to be memorized in a logical and very simple way. They relate the period numbers and/or order to the coefficients of the corresponding sublayers. Table 1 and Table 2 show the grouping of the sublayers according to energy order and period respectively.

In Table 1 and Table 2, all sub-layers are arranged in the order of stability, despite their difference. In view of the above, a relationship between order and period emerges as illustrated in Table 3.

5. Conclusions

In this work, a part of the concepts of atomistics has been demonstrated from the characteristic graph of the atom. It is a unique diagram that explains the most important concepts of the atom. The recomposition of the electronic cloud into layers, blocks, orders and periods has been illustrated by specific graphs derived from the characteristic graph of the atom. The relationship between period and order is matched in perfect agreement with the stability rule. The number of order practically ranges from 1 to 8 and that of period from 1 to 7 and for each value the different specific sub-layers are logically and easily identifiable.

Retaining Klechkowski's rule or the principle of stability, *i.e.* the arrangement of the sub-layers from "1s" to "7f" according to the level of increasing energy order, is no longer a daunting task. Today, it has been simplified and made easier so that you can start at the end or in the middle. To do this, it is sufficient to be able to count or decount from 1 to 7 or from 1 to 8.

The simplification of the establishment of the electronic structure of the elements and the proposal for a new classification model will be the subject of the next publication.

Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

References

[1] El Filali, S. (2019) Cours de CHIMIE, 2ème Partie Structure de la matière, Lycée Technique Mohamed V, Centre des classes préparatoires, Béni Mellal. https://www.cpgemaroc.com/cours/sup/phch/atomistique.pdf

[2] Decout, J.-L. (2014) CHIMIE—Structure de la matière—Chapitre 1 L'atome et ses modèles, Université Joseph Fourier. https://docplayer.fr/29196819-L-atome-et-ses-modeles.html

[3] Maghat, H. (2018) Cours atomistique/liaison chimique. Université Moulay ISMAIL, département de chimie Filière SVTU/ S1.

[4] Arnaud, P. (2001) Cours de chimie physique. 5ème édition Dunod.

[5] Prunet, R. and Prevoteau, D.B. (1994) Structure de la matière, Chimie Inorganique, DUNOD.

[6] Atkins, P.W. and De Paula, J. (2004) Chimie physique. 2ème édition Boeck.

[7] Balde, S., Barry, O. and Sylla, A. (2022) New Overview of the Energy Classification of Underlays. *Journal of Applied Mathematics and Physics*, **10**, 828-836. https://doi.org/10.4236/jamp.2022.103056

[8] Settouti, N. (2015) Reductionism in Quantum Chemistry and the Major Contradictions of the Periodic Table with Quantum Mechanics and the Role of Data Mining. Doctoral Thesis, Abou Bekr Belkaïd University of Tlemcen, Algeria. http://dspace.univ-tlemcen.dz/bitstream/112/8133/1/Le_reductionnisme_en_chimie_quantique_et_les_grandes_contradictions_du_tableau_periodique_avec_la_mecanique_quantique_et_le_role_du_data_mining.pdf