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New Overview of the Energy Classification of Underlays

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Abstract

This article focuses on a new insight into the energy classification of sublayers. In this article, the study brings out very interesting and enriching information, knowledge and knowledge in atomistics. An affine function is represented in an orthonormal frame while assimilating a point to a sublayer. This made it possible to draw up a graph integrating each of the diagrams of the known energy levels. Our results are conclusive. We can then confirm that the research hypothesis is verified.

Keywords

Atomistics, Affine Equation, Element, Quantum Numbers, Energy Level, Period, Order

1. Introduction

The curiosity of the human being is no longer to be demonstrated. Man has always tried to decipher the secrets of the elements, but the methods he used were as confused as his idea of the structure of matter [1]. Since antiquity a few years before Jesus Christ, the atomistic notion was introduced by the philosophers of the time. The search for the infinitesimal unit of matter began since the times of the Greeks, 400 years BC.

From the notion of the atom to the current classification of the elements, there have been several theories involved. Although supported by some experiments, from the great advances of the scientific revolution of the 18th century. It should be noted that most of these theories are characterized by their abstract state. This state arouses enough concern and poses serious problems for the understanding of chemistry, especially in its atomistic part, which remains and remains the gateway to any teaching relating to chemistry.

The abundance of different patterns of energy levels requires a correlation approach capable of integrating all of them. The most formidable thing of the Aufbau principle is to want to memorize in a mechanical way the order of filling of the following sub-layers: 1s, 2s, 2p, 3s, 3p, 4s, 3d, 4p, 5s, 4d, 5p, 6s, 4f, 5d, 6p, 7s, 5f, 6d, 7p, 8s.

The analysis of these problems raises concerns, attracts attention and serves as a reference to promote new scientific approaches in the field of atomistics for its better understanding.

The ambition of this work is on the one hand to develop a tool for mobilizing chemical knowledge from its development with a view to adapting it to the realities of the moment; on the other hand, to make it easier for the actors to identify the most significant facts in atomistics and to memorize them in a logical way. All these will help to develop in each other a creative imagination instead of the classic (current) methods.

This is why a team of Teacher-Researchers from the Department of CHEMISTRY, Faculty of Sciences of the Gamal Abdel Nasser University of Conakry wishes to make its modest contribution to solving the problems raised above by using the benefits of Analytical Geometry.

René DESCARTES (1596-1650), illustrious philosopher, physicist and mathematician laid the foundation for methods of solving quite complex problems by graphs formed of points, straight lines and/or circles [2].

Analytical geometry can be a much simpler method to obtain the order of the energy levels (Klechkowski's rule). Certainly, its use in the service of atomistics would make it possible to easily elucidate the different concepts of chemical language freed from any abstract theory, to memorize the most salient facts of chemistry. Each concept is represented by a line or by a point on the graph [3].

It was in 1936 that the German physicist Erwin Madelung clarified the rules for the order of filling the subshells. As a result, English sources normally cite Madelung's rule. However, Madelung offers no explanation of the importance of the sum n + l. It was not until 1962 that the Soviet agrochemist Vsevolod Mavrikievich Klechkowski (1900-1972) presented the first justification, which is why the name Klechkowski rules in French. Another name used is the Aufbau principle, after the German word Aufbau which means "construction by stacking", because this rule is used to construct the electron configuration of an atom [3].

Klechkowski's rule, also called the principle of stability, is an empirical rule allowing to find the order of filling of the subshells in order to obtain the electronic configuration of an atom in its ground state [4].

The Russian scientist KLECHKOWSKI has done a good job of describing the different energy levels of the sub-shells with several models. To better retain the sequence of filling of the sub-shells, we use an energy diagram of a polyelectronic atom, the "spaghetti rule", the Klechkowski table, the 49-square checkerboard model and the Russian model [3].

The choice of a methodology guaranteeing the effectiveness of the teaching-learning process must be a pedagogical objective well defined by the teacher. And that the teacher should be able to involve the learners and achieve the desired results. Thus, higher education must provide pedagogical approaches regarding course content through activities designed with the aim of triggering speculation on ideas and their construction and reconstruction, thus achieving active and meaningful learning [5].

The teaching of chemistry in its atomistic part requires pedagogical approaches which prioritize the dynamic (evolutionary), creative and cognitive processes of the learners and which can thus help in the construction of their own knowledge. However, learners encountered difficulties in contextualizing content such as atomistics, thus making their learning process difficult and demotivating.

Thus, learners could not understand the purpose of studying chemistry because it was complex and lacked contextualization of content. The way the content of Klechkovsky's rule was presented in textbooks hindered the presentation of teachers and the scientific interpretation of learners. Learners struggle to understand and use concepts from atomistics such as subshell energy level, period, shell, electronic structure of atoms, periodic table, etc. Because they could not consider atomistics as a tool to understand chemical phenomena; for them, it was an abstract reality. The chemist should take advantage of pre-acquired Mathematics [5].

It is envisaged to initiate a new method of interpretation of all this atomistic theory by a more concrete approach based on graphs and tables. This article is structured as follows: introduction, method, result and discussion (IMRAD).

2. Method

Use of the Equation of a Straight Line for the Atomistic Study

Atomistics is a field of abstract knowledge built using logical reasoning on concepts such as the energy level of atomic orbitals, the electronic structure of chemical elements, the period, the electronic layer, the electronic transition, etc…These different concepts of atomistics are interdependent.

A sub-layer always derives from a layer and is attached to it by its coefficient n. It is characterized by its azimuthal quantum number ℓ and the energy level of the subshell.

Any subshell is then defined by two parameters: its coefficient n and its energy order $n + \ell$. Thus a sub-layer is comparable to a point M. Mathematically a point M of a plane (Reference XOY) is defined by its coordinates x and y. M is a point of the equation: $Y = x + b$. The subshell is also analogous to the point M, whose equation: OE = $n + \ell$, where OE is the order, n and ℓ the principal and secondary quantum numbers respectively. Their similarity is as follows: M(x; y) and ns/c (n; OE). Thus Y is a function of x in the same way OE is a function of n [2].

Example: 1s (1; 1) and 7f (7; 10).

The simplest method to find graph 2 and in a very practical way is to draw a system of orthonormal axes whose origin is the nucleus of the atom, the abscissa axis is the period n (n: 1 - 7), the ordinate axis is the increasing order level of energy OE (OE: 1 - 10).

An atom is formed of some layers designated by the capital letters ranging from K to Q numbered from 1 to 7 (natural integers) "n = 1 - 7" which is nothing other than the principal quantum number. All this is summarized in Table 1 below.

A layer is formed of sub-layers designated by lowercase letters which are s, p, d, f and numbered from 0 to 3 (natural integers) "l = 0 to 3" which is nothing other than the secondary quantum number.

A sub-shell is made up of electronic cells, the quantum number also indicates the number of cells per sub-shell. If the number of cells per sub-shell or atomic orbital is designated by Nc: $Nc = 2\ell + 1$. The electronic capacity of a box is two electrons of opposite spins, the electronic capacity per orbital $Ne = 2(2\ell + 1)$. Knowing that the electronic capacitance of a layer is: $Ne/c = 2n^2$. According to the relation between n and ℓ, this equality is verifiable $2n^2 = \Sigma 2(2\ell + 1)$.

The quantum number n is an integer satisfying $n \geq 1$ while ℓ is an integer satisfying the constraint $0 \leq \ell \leq n - 1$.

In analytical geometry, the main field of graphics, lines and points are fundamental elements, which often represent processes, principles, facts and even properties to be described or explained in order to develop theories that are supposed to be more concrete (or explicit). These lines are to be identified with the breasts of the graphs, prepared to be known by interpretations which lead to laws or formulas, and sometimes even to concepts.

Using the notion of lines, we propose a method based on analytical geometry where the circle and the line play a privileged role. We are mainly interested in "the point and the line", insofar as each line can describe an atomistic concept. This is entirely in the Cartesian citation.

3. Results

3.1. Map of the Atom

By combining Table 1 & Table 2, the plan of the atom is obtained, which is as follows in Figure 1.

Table 1. Electronic layers [3].

n	1	2	3	4	5	6	7
layers	K	L	M	N	O	P	Q

Table 2. Electronic subshells [4].

l	0	1	2	3
Underlays	s	p	d	f

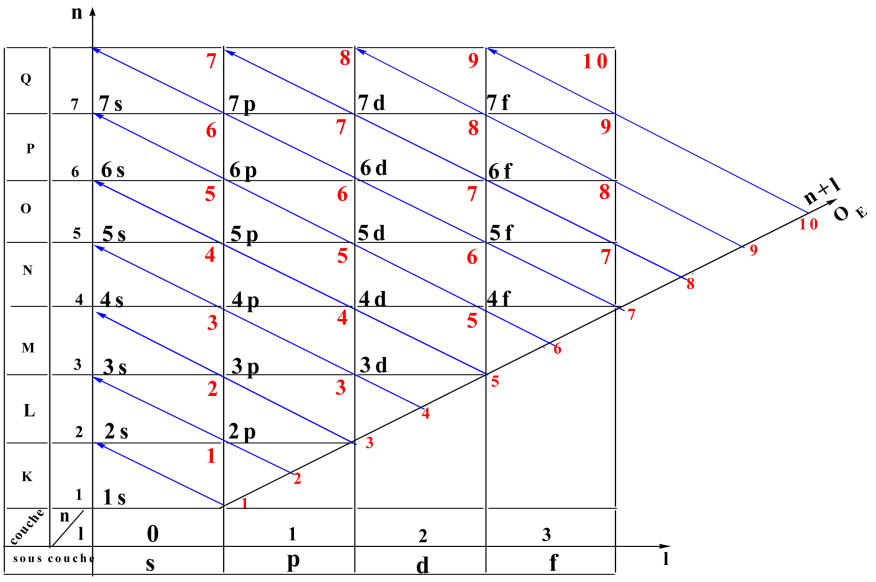

Figure 1. Blueprint of the atom.

Table 3. Numerical application of O_E.

n	1	2	3	4	5	6	7	Couches / Sous-couche
l	0	0	0	0	0	0	0	s (1 - 7)
		1	1	1	1	1	1	p (2 - 7)
			2	2	2	2	2	d (3 - 7)
				3	3	3	3	f (4 - 7)
O_E	1	2	3	4	5	6	7	s (1 - 7)
		3	4	5	6	7	8	p (3 - 8)
			5	6	7	8	9	d (5 - 9)
				7	8	9	10	f (7 - 10)

From the plane of the atom, it is possible to find the order of the energy level of each subshell (OE = $n + l$). The plan of the atom is composed of three axes namely the axis of period "n" (the layers), the axis of the orbitals "l" (the subshells) and the axis of the orders of levels of OE energy.

This plan confirms that a subshell is characterized by two values: its coefficient "n" and its order of energy level "O_E", which makes it a point similar to that M of an XOY plane in a system of orthonormal axes.

Example:

1s - 7s: 1s (1; 1) 7s (7; 7);

2p - 7p: 2p (2; 3) 7p (7; 8);

3d - 7d: 3d (3; 5) 7d (7; 9);

4f - 7f: 4f (4; 7) 7f (7; 10).

Therefore the atom can be characterized by a graph. The origin of such a graph would be the nucleus (N) of the atom; the ordinate would be the order of the energy level (O_E) and the abscissa the period (n).

3.2. Study and Graphical Representation of the Equation $O_E = n + l$

- Correlation table

For precise values of n = 1 to 7 and l = 0 to 3 respectively for each layer and sublayer, the solution set O_E = 1 to 10 of this equation is recorded in the numerical application table (Table 3) above:

The graph resulting from this numerical application is characteristic of the atom. The order O_E evolves from 1 to 10 and each value includes a certain number of sub-layers for O_E = 1 and 2: there is only one sub-layer per value, for O_E = 3 and 4 there are 2 sub-layers, for the values 5 and 6 the number of sub-layers is three, the value 7 is composed of a maximum of four sub-layers. At 8 the number of sublayers drops, orders from here are incomplete.

- The representation of the characteristic graph of the atom:

This graph is presented in a system of orthonormal axes of the "n N O_E" type (n the period, N the kernel, origin of the axes and OE increasing order of the energy level: the ordinate). It is a question of reproducing the pedagogical approach. It amounts to placing all the subshells in an orthonormal reference $O_E = f(n)$: (Figure 2).

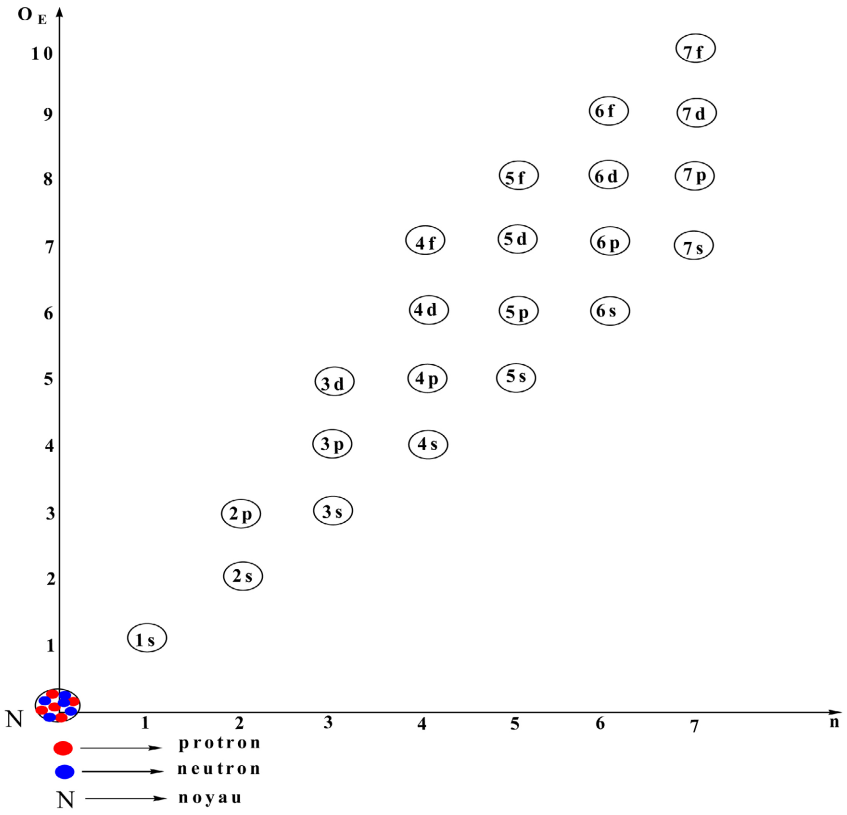

Figure 2. Arrangement of sublayers in the orthonormal reference.

This graphic logically describes the positioning of each element of the electronic cloud. The sub-layers are points of the electronic cloud and their grouping in layers, in periods, in blocks, in orders is illustrated by this diagram. It better expresses the relationship between the dimensions of the nucleus and the electronic cloud (Figure 3).

The graph characterizing the atom is a new diagram of the energy level. It integrates the different diagrams known from the literature such as the KLECHKOWSKY rule diagram, the Russian model, the energy diagram of a poly-electronic atom, the 49-square checkerboard model, etc. It absolutely expresses the idea of Aufbau (building by stacking).

4. Discussion

For each O_E value, the corresponding sublayers are indicated. And their coefficients are related to the value of O_E. For ns subshells, $O_E = n$.

For the other components (sub-shells), their coefficients are counted from the value of O_E up to the admitted values 1s, 2p, 3d and 4f.

An order is structured as follows: $(n-3)$ f, $(n-2)$ d, $(n-1)$ p and ns. This makes it possible to logically identify the sublayers of each order. Practically O_E goes from 1 to 8 (8 is incomplete). It is enough to count from 1 to 8 to establish the Rule of stability (Table 4).

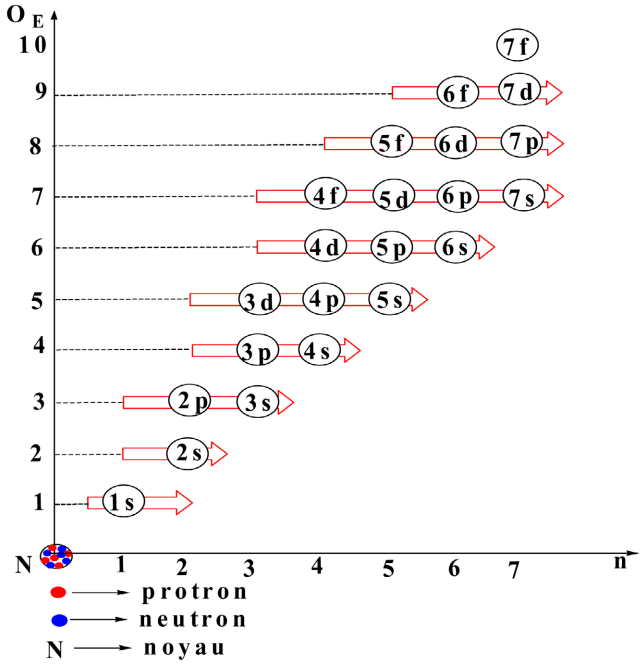

Figure 3. New energy level arrangement of atomic orbitals.

Table 4. Appearance of the sub-layers according to the orders of energy.

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 …

5. Conclusion

Our work made it possible to sequence the sublayers in order. This makes it possible to memorize them logically, knowing that the coefficient of each sub-layer derives from the number of the order of energy. The characteristic graph of the atom constitutes a diagram of the level of energy which correlates with all the diagrams of the literature. On its own, it can illustrate each of the concepts of the classification of elements and their electronic structure. This schema will make it possible to specify the classifications of the elements. In the literature, not every classification can be periodic [6].

Conflicts of Interest

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

Futures Works [7]

In this paper, subshell energy level results confirming the use of an affine equation have been provided. We hope to provide a rigorous proof of the terminology of atomistics using the equation of a straight line in the near future, such as the electronic structure of chemical elements, the methods of illustrations of the different classifications of chemical elements to order and to period, the presentation of the layers, of the periods and of the electronic jump.

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Abbreviations and Acronyms

The following abbreviations are used in this document:

IMRAD: introduction, Method, Result And Discussion.

KLMNOPQ: electronic shells appearing respectively when $n = 1, \ldots, n = 7$ (Table 1).

ℓ: secondary or azimuthal quantum number $0 \leq \ell \leq n - 1$.

M(x; y): point M in an orthonormal frame of coordinates x and y.

n: principal quantum number where $n \geq 1$.

Nc: number of atomic orbitals per subshell $Nc = 2\ell + 1$.

Ne/s/c: number of electrons per subshell $Ne/s/c = 2(2\ell + 1)$.

Ne/c: number of electrons per shell $Ne/c = 2n^2$.

O_E: energy order or energy level of a subshell $O_E = n + \ell$.

spdf: subshells appearing respectively when $\ell = 0, \ldots, \ell = 3$.

XOY: orthonormal reference with axis OX (axis of abscissa), OY (axis of ordinate) and origin O.

$Y = x + b$: affine equation of a straight line.