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Research Article

INTERPRETATION AND REPRESENTATION OF THE THEORIES OF WERNER, PAULING, HUND'S RULES AND MOELLER'S DIAGRAM, IN THE ANALYSIS OF ANOMALIES FOR A PROFESSIONAL INTRODUCTORY EDUCATIONAL LEVEL

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Abstract

The purpose of this documentary and explanatory research work is for didactic purposes, professional improvement and contribution in the area of Chemistry. The didactic method with all certainty to teach any topic, of any subject, of any level and in any field is Teaching to Think and Analogical; to learn it requires developing cognitive skills in students. The topic presented is an interpreted and represented mathematical strategy of Hund's rules, to analyze the "anomalies" that apparently do not have a pattern, they are also based on the theories of Pauling and Werner, without these theories it would not be possible to justify the behavior of certain representative elements similar to anomaly behavior. When carrying out an analysis, it can be concluded that, being different, all anomalies have a general and a particular attribute; the first is that all the anomalies coincide in that the valence electron is responsible for seeking stability in the last orbital of the electron configuration, and the second depends on the location of the valence electron to which this last electron belongs in the configuration electronics of each element, making this the difference in each anomaly. In addition, an update is added to the proposal for a new design of the Periodic Table, presented in a previous article by the author, hence it is concluded with complete certainty that in the new proposed design a new pattern was identified that organizes the elements in their basal state by the Moeller Diagram.

Keywords: Anomalies, Abilities, Pattern, Valence, Strategy.

INTRODUCTION

An analysis of the presented topic is carried out because to date there is no apparent pattern that justifies the behavior of certain representative elements and anomalies; It is based on Werner's theories because primary and secondary valences will be used, Pauling's theory because it is essential in the electronic configuration of each element, Hund's rules because it will be the mathematical interpretation of the intervals in which anomalies occur, and Moeller's diagram because it is interpreted vertically, horizontally and diagonally; The latter is the way it has been used for years to write the electronic configuration of the elements, the vertical form orders the blocks to the left and right in the new design of the Periodic Table proposed by the author, the horizontal form will indicate the number of orbitals present per level and the coordination nucleus, according to the author. To distinguish everything that is stated, a color code is used to highlight what the student must identify in the model examples, for this it is required at all times to develop elementary cognitive skills such as observing, relating, comparing, classifying and describing. By mastering these skills in the model examples, the student must develop superior cognitive skills such as interpreting and representing in any other element what was learned in this topic. The fundamentals that support this study are the following:

The concept of oxidation number is a periodic property associated with the electronic configuration "it is the gain or loss of electrons if it is considered that the bonding electrons are associated with the most electronegative atom" (Valenzuela Calahorro, 1995).

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"The concept of *primary valence* as *the oxidation state or number* and *secondary valence* as *the coordination number*, in recognition of Werner's Theory, for coordinated compounds in Organic Chemistry (Tejada, Acevedo, & Gattas, 2014) (Moeller, 1994)". "The formation of coordination compounds is not a phenomenon limited to atoms of elements of the (d) or (f) block, but also of the representative block, such as Magnesium and Aluminum". "According to the electronic structure, the central atom can form several bonds, this number of bonds is known as *the coordination number*" (Alfonso Parada, 2012). Werner's theory (1893) states that: "*The primary valence*, based on the number of electrons that the atom loses to form the metal ion, and *the secondary valence* that is responsible for the bond with other compounds , called ligands, to the central metal ion. " (Tejada, Acevedo, & Gattas, 2014). "The central atom called also *coordination nucleus* corresponds mainly to metallic ions, (although it can be cation, neutral atom or anion), which act as Lewis acids, surrounded by molecules or anions called ligands, which act as Lewis bases providing electronic pairs. " (Alfonso Parada, 2012) (see Figure 1). The *Pauling Hybridization* concept: "at the moment of combining, the atoms reach a state of excitation, as a consequence of the energy they gain; in such a state, some electrons jump from a lower orbital to an immediately higher one, causing a recombination of these and the formation of a new set of hybrid atomic orbitals "(Alfonso Parada, 2012). The fundamentals that support the "anomalies" are: 1.) The electrons to keep the balance jump from one orbital to another and do so in orbitals with the same energy and higher level (Origel, 2003) and this is very easily verified by applying the formula (n + l) (Jaramillo Sanchez, 2004), as occurs with elements where the intervals are: (d <5) and (f <7). 2.) "Hund's rule assigns electrons to the largest possible number of orbitals in a sub-layer justifies the following expressions: it is said that: a sub-layer is full if 2 (2l + 1) electrons have been assigned to

it and that it is half full if (2l + 1) electrons have been assigned ”(Picado & Milton, 2004), with the same formula it is stated that“ As the orbital angular momentum has, in addition to magnitude, (2l + 1) possible orientations in space …. ” (Sharpe, 1993). 3.) With the same formula we find “We know that for each energy sublevel, there are a number (2l + 1) of possible orbitals, therefore the sublevel (s) has only one orbital, the sublevel (p) will have three orientations… ”4.) According to Paulling's Principle:“ In an atom there cannot be two electrons with the four equal quantum numbers ”,“ The maximum number of electrons for the orbital (s) is 2, for the orbital (p) it is 6, for the orbital (d) it is 10 and for the orbital (f) it is 14 ”(Tejón, García, Jimenez, & Guerrero, 2006)“ The outermost electron of each one of the elements of this period is less firmly bound than the outermost electron of the corresponding element of the previous period (Origel, 2003). 6.) For the transition series they can lose a high number of electrons without reaching the inert configuration, due to their valence variability and the ions have partially occupied the (d) orbitals and others with complete electronic levels d^{10}” (Gutierrez Rios, 1985) “only halogens and elements of the oxygen group act as negative ions”. 7.) "The oxidation states for block (f) in Actinides are (+3) normally because they are ionic salts, the Lanthanides are more radioactive " (Dickerson, Harry, Darensbourg, & Darensbourg, 1992) "generally, the states of oxidation diminish as its atomic number increases)” The ionization process is not an anomaly but because of the electronic configuration it is taught and when it is taught it is usually said that "electrons are lost" when forming cations or "they gain electrons when forming anions"; as well as for the case of Iron.) “the interactions of the electrons alter the energy of the different orbitals when the difference is small and alters the indicated order” also “the indicated facts have no impact on the chemical properties of the corresponding elements” (Gutierrez Rios, 1985). “Electrons occupy the orbitals in such a way as to minimize the total energy of an atom, maximizing attractions and minimizing repulsions according to Pauling's principle and Hund's rule” (Attkins & Jones, 2007).

The concept of *Hybridization* was born in 1931, “when Mr. Pauling explains that Carbon theoretically only presents two possibilities to form bonds when experimentally it does so with four, ensuring that an electron is promoted to the unoccupied (pz) orbital; observing in an X-ray experiment, this justifies the organic molecular geometry” (Lanchero Barrios, 2013). The concept of *sphere* "is a region very close to the *coordination nucleus* where it is feasible for the electrons of the ligand atoms to interact with *unoccupied orbitals* of the Lewis acid species" (Alfonso Parada, 2012) (Moeller, 1994). The *coordination nucleus* concept is "the central atom and corresponds to ions, neutral atom or anion, which act as Lewis acids surrounded by molecules or anions" (Alfonso Parada, 2012) (see Figure 1); this group at each level is a key element for the topic of Anomalies and Hybridization, offers the ability to form links and therefore compounds that have the elements per level and we can see it with the behavior of Fluorine, Chlorine, Thorium and Beryllium, the latter having a *coordination nucleus* (s, p) will complete only four, it will never comply with the octet rule, since only two electrons are placed in each orbital and their coordination number is two for Beryllium; Fluorine and Chlorine (-1) they will complete eight because they have two electrons in (s) and six electrons in (p) when joining with another atom, its coordination number is four for both elements, but Fluorine differs from Chlorine as it has a variable valence because it is at level three, that is, it can jump its valence electrons to an orbital (d) because its *coordination nucleus* is (s, p , d) unlike Fluorine where its *coordination nucleus* is (s, p) thus forming more compounds than Fluorine ClF_3, and Nitrogen, of which only NCl_3 is known; the following is the justification for Pauling's valence theory; "In the elements of the following periods n> 2 there are (d) orbitals, so there may be a greater number of unpaired electrons than in the previous level…." (Gutierrez Rios, 1985) and also justifies the author's interpretation regarding the coordination nucleus of the central atom. (Lima, Tonydandel *et al.,* 2017) (see Figure 1).

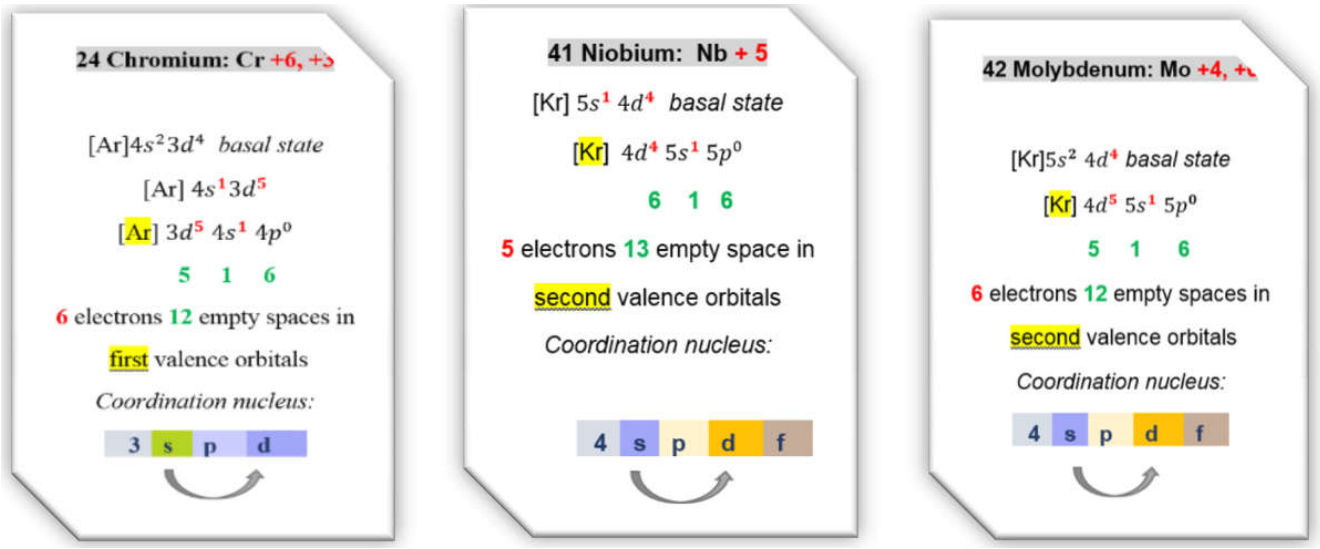
METHODOLOGY

The teaching method is with all certainty “Teaching to Think (Swartz, 2019), Analytical and Analogical, and for learning it is recommended to develop cognitive skills (Woolfook, 2011) by applying color coding in activities for upper initial level students. . To achieve this documentary and explanatory research work, the hypothetical-deductive method was applied, which consists of: 1.) Five phenomena that occur in the electronic configuration of the block elements (d) and (f) are observed, and they are identified as "anomalies" or other synonyms without an apparent pattern that identifies them: a.) Jump of the last electron in an interval ($d \leq 5$) particular cases: Cr, Nb, Mo (see figure 2); b.) Jump of the last electron in an interval ($d \leq 10$) particular cases: Cu, Ag, Au, Pt. Pd, Rh, Ru (see figure 3); c.) Having an electron in orbital ($6d^1$) creates instability, *to avoid this the last electron is located in the next orbital (*$7p^1$) in an interval ($d \leq 5$). Unique cases: Lawrencium (Lr) (see Figure. 4) in block (d) and Thoriumin block (f) (see Figure5); d.) Having one or two electrons in the last orbital or pattern creates instability, *for this a change of orbital occurs*, the electrons try to reach equilibrium without achieving it. Block attribute (f) in i*nterval* ($f \leq 7$) particular cases: Th, La (see figure 5); e.) There is no exponent 8, the electrons distribute the last electron to a next orbital to maintain the equilibrium in orbital ($4f^8$) and ($5f^8$); cases: Gd, Cm. ($f = 7$). Starting from $4f^9 or\ 5f^9$ there are no longer changes in an interval ($f \leq 14$). 2.) A hypothesis is proposed: Is it possible to find a mathematical didactic strategy that identifies when and for what these phenomena occur? 3.) Interpret and represent Hund's rules as intervals, which define when and for what these phenomena occur and to relate the foundations already established to justify the “anomalies”. 4.) It is generalized that the "anomalies" are phenomena that have a foundation established for years ago and by identifying *the intervals* it can be affirmed and verified that the "anomalies" occur in the elements of block (d) and (f) mainly to achieve stability, and depends on the location of the valence electron to identify itself in some category. In the analysis of “anomalies, it starts from experimental data (Attkins & Jones, 2007) since the elements of Nature have a different behavior than the theoretical, in practice according to the scientists this behavior is called Anomalies; there are the fundamentals that explain the why of these anomalies, it is analyzed why and when these intervals occur; Therefore, it is intended to solve these problems with the application of didactic strategies to analyze and justify them. “The term anomaly, refers to a difference between the electronic configuration that is attributed to the element, which is expected to be present if the Aufbau principle is followed; but it does not mean that there is an abnormality. " (Attkins & Jones, 2007) (Picado & Milton, 2004).

Model cases	Interpretation	Representation of the coordination nucleus	Analogy
Beryllium s p Fluorine	Beryllium is located in the orbital (s) and can jump an electron to the (p) orbital to hybridize, while Fluorine is occupying (p) orbital, it no longer has space to hybridize, so this element cannot form more compounds than the space it has to offer: an electron.	n = 2 Coordination nucleus: 2 s p	If you have two bedrooms, you can move from one to another, but you cannot move to a third bedroom because you do not have one.
Chlorine p d Lawrencium	Chlorine is located in the orbital (p) and can jump the orbital (d) to hybridize, while Lawrencium is in orbital (d) and jumps an electron to (p) orbital, this being a changer of orbital, an electron creates instability, also in level =3 there is no space (f); an anomaly.	n = 3 Coordination nucleus: 3 s p d	If you have three bedrooms, you can move from one to another, but you cannot move to a fourth bedroom because you do not have one.
d f Uranium Thorium Cerium Actinium Lanthanum,	Having one or two electrons creates instability like Lanthanum, Actinium and Thorium it changes orbital from (f) to (d) because after (f) there are no (g) orbitals and therefore block (g) so they jump towards (d). Protactinium, Uranium, Neptunium, Gadolinium, are in an orbital in (f) and it does no change it, but rather it distributes one electron to an orbital (d), this being an anomaly.	n = 5 Coordination nucleus: 4 s p d f 5 s p d f	If you have four bedrooms, you can move from one to another, but you cannot move to a fifth bedroom because you do not have one.

Source:*Own authorship, 2020.*

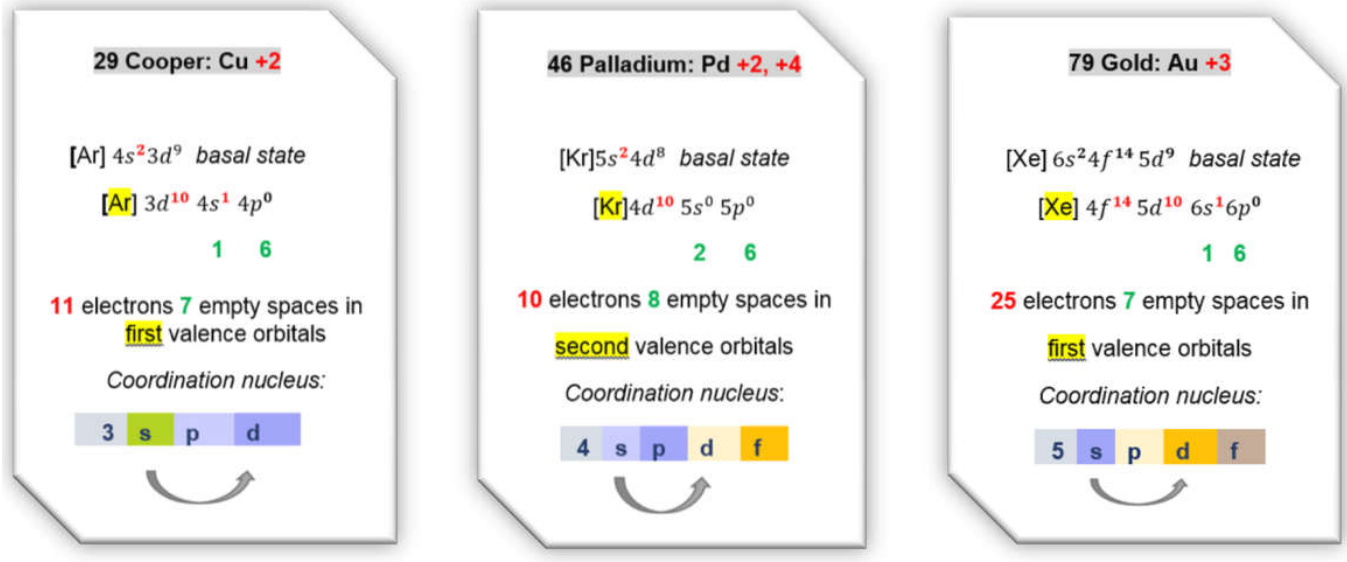
Figure 1. Interpretation and representation of the postulate of Hund's rule and the coordination nucleus of the central atom of Werner's theory and Pauling's Hybridization



Source:*Own authorship, 2020.*

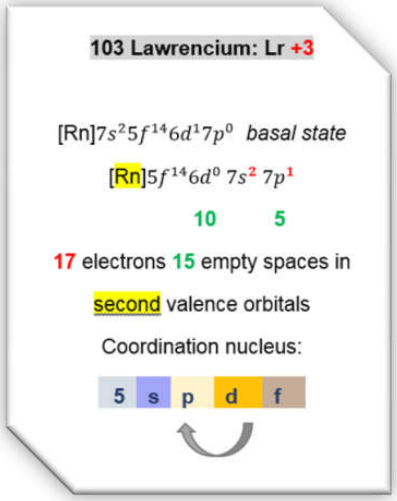
Figure 2. Anomaly 1

The "anomalies" are originated from experimental data reported by scientists and will be analyzed in the following sections. The first "anomaly" to be analyzed is the one where: the last electron jumps to another orbital *to achieve stability and favor oxidation states*; When achieving stability in a semi-full layer, this occurs in an *interval* ($d \leq 5$). Cases: Nb, Mo, Cr (Origel, 2003) and in a semi-full layer ($d = 5$) we have: Re, Tc, Mn, in this interval it is in equilibrium. The second anomaly is the electron jump *to achieve equilibrium* in an interval ($d \leq 10$), the valence electron jumps to complete orbital (d) to ten electrons seeking equilibrium even though it is not achieved; particular cases: Cu, Ru, Rh, Pd, Ag, Pt, Au; they are in total equilibrium ($d = 10$) we have: Cd, Zn, Hg, Cn; In the particular case of Palladium, the shape of the orbital disappears ($4s^2$) where these two electrons "are not lost", but are *relocated* in the next orbital to *achieve equilibrium* ($4d^8$), is achieved the total equilibrium in orbital (d) and the second valence ([Kr] $4d^{10}5s^25p^6$) is started. The third anomaly consists of having an electron in orbital ($6d^1$) creates instability because it is further away from the nucleus and *to avoid it, the last electron is located in the previous orbital* ($7p^1$) in a criterion ($d \leq 5$). Unique case: Lawrencium (Lr) *orbitals* ($6d^1$to$7p^1$).



Source:*Own authorship, 2020.*

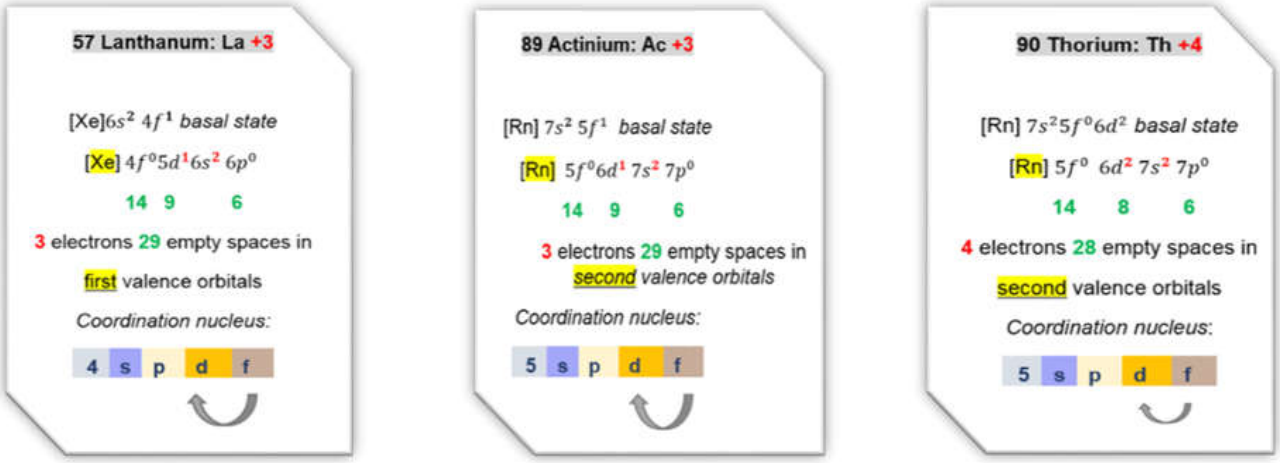
Figure 3. Anomaly 2



Source:*Own authorship, 2020.*

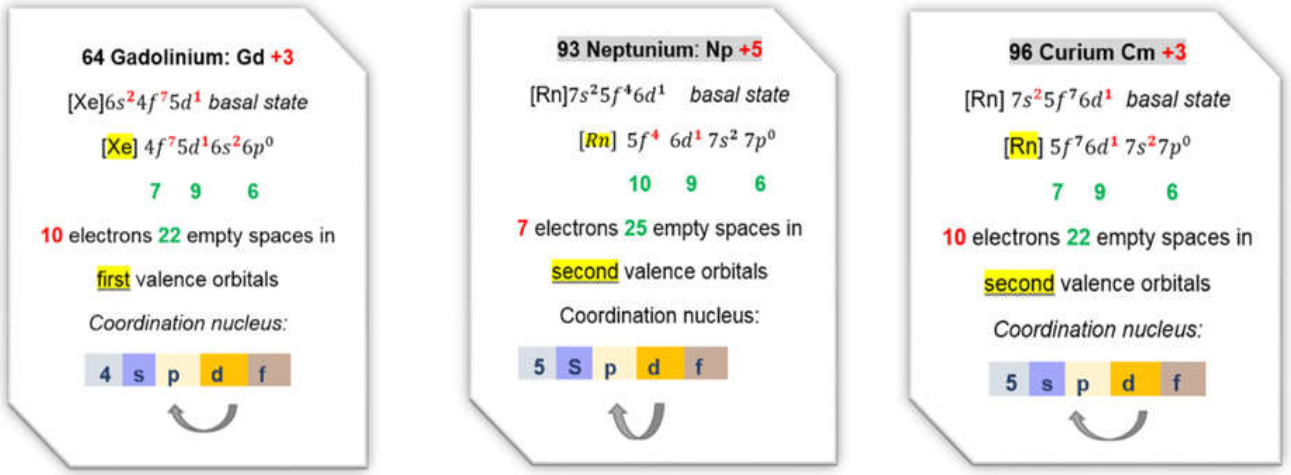
Figure 4. Anomaly 3

The fourth anomaly consists of having one or two electrons in the last orbital or pattern creates instability because it is far from the nucleus, *for this, a change of orbital occurs*, the electrons try to reach equilibrium without achieving it. Attribute of block (f) in *criterion* ($f \leq 7$) particular cases: Ac ($5f^1 to 6d^1$), Th ($5f^1 to 6d^1$), La ($4f^1 to 5d^1$) (Gutierrez Rios, 1985). "Having one or two electrons (n) in an orbital ($5d^n$) or ($6d^n$) creates instability, so the electron jumps to an inner orbital, for two reasons: one because it does not exist in current elements with (g) orbitals, if they existed there would be block (g) in the Periodic Table and therefore the coordination nucleus is (s, p, d) for block (d); it has been thought that they must be occupying the same place that actually corresponds to Lutetium (Lu) and Lawrencium (Lr) "because they have in their last orbital ($d^1 y d^2$) (Scerri, 2019) but it is the same phenomenon only that these elements are of orbital (f) and also jump to an inner orbital for the same reasons. The foundation is found in Hund rules (Jaramillo Sanchez, 2004) (Origel, 2003) (Valenzuela Calahorro, 1995) (Gutierrez Rios, 1985). In the Lanthanide group, the electron jumps from the *orbital* ($4f^1$) to the ($5d^1$) in the case of Lanthanum, since having one or two electrons creates instability; for Actinides: Actinium, $6d^1$ instead of $5f^1$; Thorio $6d^2$ instead of $5f^2$; by Hund rules (Valenzuela Calahorro, 1995). For an element of block (f) there is no other block (g) in the Periodic Table, that is, there is no more space to jump, there is neither an orbital (g) nor a block (g) in the Periodic Table, so the electron is located in the previous orbital, (see Fig. 1, 5) according to the author based on the foundation of the bond theory (Gutierrez Rios, 1985). The fifth is not an anomaly, it is a reference, where it is observed that they totally achieve equilibrium, particular cases: Europium (Eu), Americium (Am) in (f = 7). The sixth anomaly is that there is no exponent 8, the electrons distribute the last electron to a next orbital to maintain equilibrium instead of presenting the orbital ($4f^8$) and ($5f^8$); corresponds to a $6d^8$ and does not present it but$6d^9$ to approach equilibrium in a criterion ($d \leq 10$). In block ($f \geq 8$): Cm should be ($5f^8$), however it distributes its last electron in ($5f^7 6d^1$), Gd should be ($4f^8$), however it distributes its last electron in ($4f^7 5d^1$), Neptunium should be ($5f^5$) and an electron is distributed to ($6d^1$); these elements manage to maintain equilibrium at ($f = 7$). From $4f^9$ *or* $5f^9$ there are no longer changes in an interval ($f \leq 14$) or ($9 \leq f \leq 14$). (see Figure 5, 6).



Source:*Own authorship, 2020.*

Figure 5. Anomaly 4

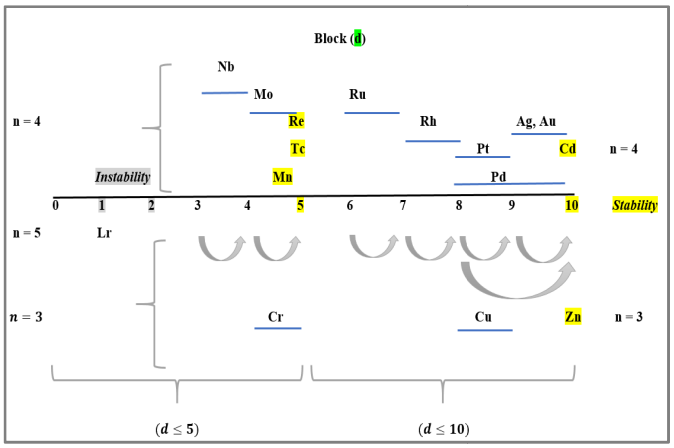


Source:*Own authorship, 2020.*

Figure 6. Anomaly 5

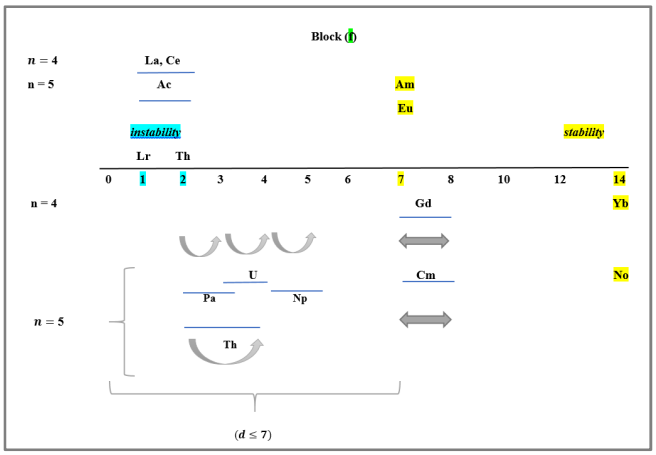
DISCUSSION

The identified intervals based on Hund's rules are a mathematical didactic strategy that allows us to analyze the elements for study and to be able to visualize and identify the "anomalies", "paradoxes", "irregularities" or "exceptions" that some elements of the block (d) and (f) mainly shows; to understand behaviors different from the theoretical. In the following figures 7 and 8, you can see the jump of electrons towards equilibrium in all anomaly cases, it depends on the location of the last electron that makes the difference. Figure 9 shows the relationship of Werner's theories and their concepts of primary, secondary valence, coordination nucleus; Pauling's theories in filling of electrons in the orbitals; Hund's postulates represented with the intervals; in Moeller diagram, the nucleus of coordination is identified in color. After completing this topic, the skills in the acquired knowledge can be applied: the student must recognize the pattern that is the last orbital of the last level in the electronic configuration, which places each element in its basal state in its box in the Periodic table; Recognizing the ability to form compounds depends on the level at which the central atom is located and, therefore, on its coordination nucleus, for this it is enough to interpret the Moeller diagram by level and it will indicate the orbitals found at that level. Recognize Hund's rules which are represented by the intervals in which anomalies occur, identify the location of the valence electron, which differentiates the anomalies. Differentiate the exponents in the electron configuration which indicate the number of electrons or negative charges (the same amount of positive charges) from the exponents in the molecular geometry indicate the number of occupied orbitals. Identify the first of the second valence where there are unoccupied orbitals, observe that the ligands participate with their two electrons, such as diatomic molecules or molecules with free pairs. Recognize the limit of when it is said first or second valence, observing that after Helium, Argon and Xenon is first valence, after Neon, Krypton and Radon it is second valence. Interpret the theories involved in the subject; differentiate the worked examples. You can also answer some questions: Why do electrons jump in some elements and no jumping is required in others?. In the elements that do not require jumping, it is because the valence electrons act so that a covalent bond occurs (one to one of each element as in the case of sodium and chlorine (-1) to form sodium chloride; in the case that they have to jump like Beryllium is because it is saturated and because being at level 2 and block (s), it has orbital (s) and has space in orbital (p) to form a bond with chlorine and form beryllium chloride; in level 3,



Source:Own authorship, 2020.

Figure 7. Block (d) Anomaly Scheme



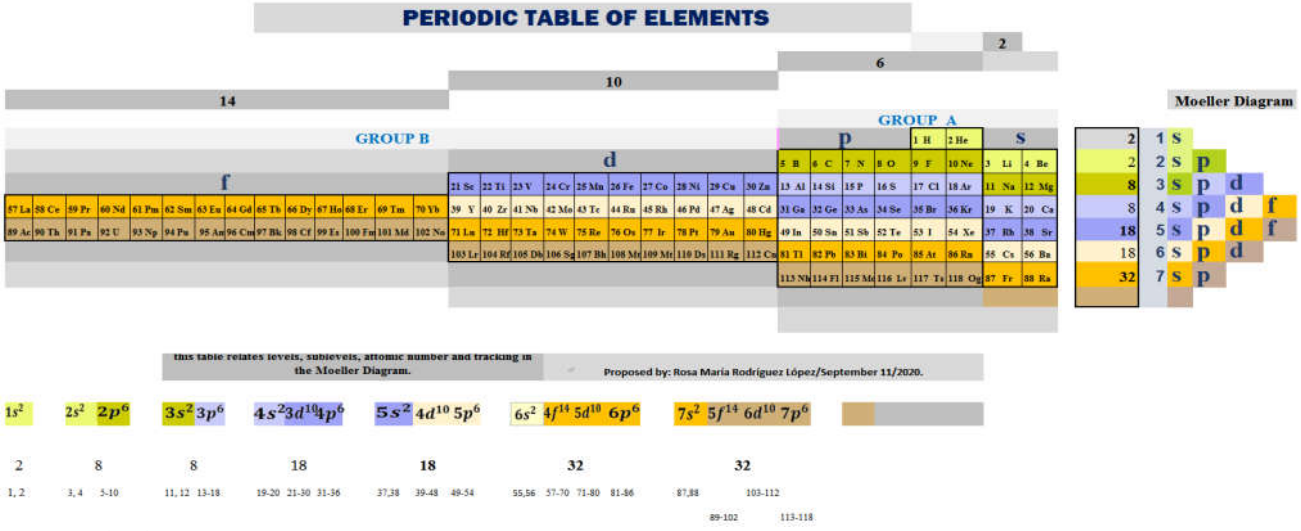
Source:Own authorship, 2020.

Figure 8. Block (f) Anomaly Scheme

Element 26 Iron Fe +2, +3 [Ar] $4s^2 3d^6$ state basal		$3d^5$ "three electrons are lost" 5 electrons 11 holes in first valence	
Interpretation	*Ionization*	*Molecular geometry: d^2sp^3*	*Molecular geometry: sp^3d^2*
Three electrons are lost from the central atom to make it $4s^0$ orbital empty, by leaving the orbital $4s^0$; the first valence $4p^0$is opened; the 3d orbital achieves equilibrium as requirement to be able to use the second valence if required. The equilibrium for orbital (d) is five or ten, stated by Pauling. Only complexes the configurations d^3, d^4, d^5, d^6 can have high and low spin (Gutierrez Rios, 1985) low spin d^5, d^6 configurations are more stable than high spin complexes (Origel Leslie, 2003)	Fe^{+3} [Ar] $3d^5\ 4s^2\ 4p^0\ 4d^0$ 5 6 Valence electrons: $4s^2 3d^6$ $3e$ *First valence:* $4s^0\ 4p^0$ *Second valence:* $4d^0$ Coordination number: 6	$[Fe(CN)_6]^{-3}$: **Low spin model:** $[3d^5\ 3d^4\ 4s^2\ 4p^6]$ CN CN CN CN CN CN	$[FeF_6]^{-3}$: **High spin model:** $[3d^5\ 4s^2\ 4p^6\ 4d^2]$ F F F F F F
$[\pm 3 - 8] = 5$ ..... $3d^5$	0 1 2 3 4 5 6 7 8 Interval graph		3 s p d Coordination nucleus

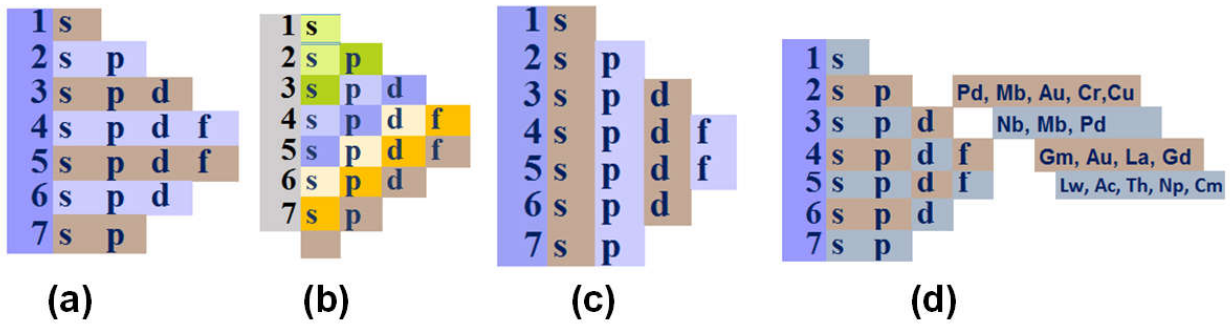
Source:Own authorship, 2020.

Figure 9. Interpretation and representation of Werner, Pauling theory, Hund's postulates and Moeller diagram in block model element (d)



Source:Own authorship, 2020.

Figure 10. Update to the proposed new design of the Periodic Table



Source:*Own authorship, 2020.*

Figure 11. Interpretation and representation of Moeller diagram

block (d) there is more space and these elements have the option of forming more compounds. Why do the electrons come out and "get lost"? As in the case of Iron, three electrons come out and three molecules bond in the place unoccupied with its two electrons each in valence orbitals, if necessary, the first valence and / or second valence are used depending on the number of binders. Why are there elements that do not comply with the Octet rule? Because it depends on their number coordination, in each orbital only two electrons have space and they are distributed two by two; observe, relate and compare Beryllium, Manganese, Boron, Aluminum, Chlorine, among others. Why does Chlorine (-3, -5, -7) behave as an element of block (d)? because it is in level 3 where there are orbitals (s, p, d) and in that same level is the block (d), Chlorine being in (p) has space to jump in (d). Why does Chromium instead of $4s^2\ 3d^4$ have $4s^1 3d^5$ and other anomalies? Because as already analyzed, the last electron oversees seeking equilibrium. It should be clear that the elements follow the Moeller diagram in their basal state organized in a Periodic Table and the anomalies observed by the scientists in the experimental part they actually do have an observable pattern or behavior in the figures 7 and 8 presented before. As an update to the first article presented by the author (Rodríguez López, 2020), it is reaffirmed that the Moeller diagram indicates the location of the elements in their basal state by identifying the pattern in the electronic configuration in *diagonal* order (Groosvenor Cooper, 1976) (see figures 10,11).

(a) The elements in the basal state are located in the Periodic Table by a pattern identified in the electronic configuration determined by the Moeller Diagram.
(b) The elements in the activated state are identified as Anomalies with their own pattern that is based on Hund's postulates, and consists of the valence electrons jumping to a.) Achieve equilibrium in the (d) and (f) orbital.
(c) The vertical sequence tells us the order in which the blocks in the Periodic Table are arranged to the left and to the right.
(d) The presented sequence indicates the last first and second valence orbitals with some examples.

CONCLUSION

- Developing basic and superior cognitive skills is how this research work has been achieved and it is recommended to develop them in students in any area of knowledge.
- Each element in its basal state has its location in the Periodic Table according to the Moeller diagram; The report by scientists regarding anomalies is due to the
- Anomalies have a general and a particular objective: the first is to find the equilibrium where the last valence electron acts. The second objective is that the location or interval that the valence electron is found depends on to select the interval in how to achieve said stability.
- It has been essential to understand the theories of Werner, Paulling, Hund's postulates and Moeller's diagram in order to document the analysis of Anomalies.
- The unoccupied orbitals in the first valence are precursors to enable the second valence where the ligands enter; In addition, the electrons in orbitals (d) try to maintain equilibrium, always completing with ligands, according to the author.
- For years the Moeller diagram has been considered a simple mnemonic rule and it has been taught that it is only used diagonally to write the electron configuration, when this rule is the key to understanding the organization of the Periodic Table, the nucleus of coordination, and the behavior of valences, in the present, according to the author.
- It is expected to have achieved the objective of facilitating the learning of the subject and the acceptance of the scientific community.

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