How the Even-Odd Rule, by Defining Electrons Pairs and Charge Positions, Can Be Used as a Substitute to the Langmuir-Octet Rule in Understanding Interconnections between Atoms in Ions and Molecules

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Abstract

In the course of time, numerous rules were proposed to predict how atoms connect through covalent bonds. Based on the classification of elements in the periodic table, the *rule of eight* was first proposed to draw formulas of organic compounds. The later named *octet rule* exhibited shortcomings when applied to inorganic compounds. Another rule, the *rule of two*, using covalent bonds between atoms, was proposed as an attempt to unify description of organic and inorganic molecules. This rule unfortunately never managed to expand the field of application of the *octet rule* to inorganic compounds. In order to conciliate organic and inorganic compounds, the recently put forward *even-odd* and the *isoelectronicity rules* suggest the creation of one group of compounds with pairs of electrons. These rules compass the *rule of two* for covalent bonds as well as the *octet rule* for organic compounds and suggest transforming bonds of multi-bonded compounds in order to unify representations of both groups of compounds. The aim of the present paper is fourfold: to extend the *rule of two* to every atom shells; to replace the well-known *octet rule* by the *even-odd rule*; to apply the *isoelectronicity rule* to each atom and to reduce the influence range of the charge of an atom in a compound. According to both rules, the drawing of one atom with its single-covalent bonds is described with electron pairs and charge positions. To illustrate the rules, they are applied to 3D configurations of clusters.

Keywords

1. Introduction

Abegg, Lewis and Langmuir [1]-[3] have suggested a procedure to represent molecules with single or multiple connections between atoms. They also put forward a rule known as the *octet rule* to obtain valid chemical structures of organic compounds. Molecules like CH4, NH3, H2O and HCl are known compounds of this family, with eight electrons in the valence shell around the central atom. In CH4, the atom of carbon possesses 4 valence electrons: it can be connected to four atoms of hydrogen by means of eight electrons forming covalent bonds. A few incompatible molecules had however already been discovered, like BH3 or BeH2. Considering these molecules, Lewis introduced the *rule of two* [4]. This *rule of two* suggests that electrons combine in pairs, *i.e.* covalent bonds, to make each connection in organic and inorganic compounds. The *rule of two* seems to have a wider field of application [4]. Unfortunately, the *rule of two* does not expand the application field of the *octet rule* [5].

A rule named *even-odd rule* has recently been proposed [6]. This rule was validated for a large number of known ions and molecules [6] [7]. Based on these early validations, the *even-odd rule* has suggested modifying multi-bonded compounds into single-bonded compounds [8]. As a consequence, compounds classically multi-bonded and modified with the *even-odd rule*, are encompassed with all the other single-bonded molecules [8]. At the same time, an *isoelectronicity rule* has been defined and applied to single-bonded ions and molecules [9].

The aim of the present article is to submit a drawing procedure of ions and molecules, by describing how to apply the *even-odd* and the *isoelectronic rules* to single-bonded compounds. Both rules are firstly defined as local rules to determine the calculation procedure of the even number of electrons in each atom shell. In the process, the author takes example of each possible element of the main group of the periodic table, along with their bonding conditions and charge positions. 3D drawings illustrate then the *even-odd rule* applicability. Several points are finally discussed such as the importance of the number of electrons in the atom shells and the local nature of both rules when applied to charged or uncharged atoms.

2. The Even-Odd Rule for an Atom in Ions and Molecules

The even-odd rule indicates in which of the three atom shells, electrons are located: the inner shell, the inactive shell and the covalent shell. It reads as follows:
- Each element of the periodic table that is not part of a compound:
  - is electrically neutral with a number of positive charges and the same number of electrons,
  - is composed of a nucleus, where positive charges are located,
  - possesses around the nucleus, an inner shell composed of an even number of electrons,
  - possesses a valence shell with a number of electrons equal to the valence number of the atom, as defined in the periodic table,
  - has no covalent shell: it is not covalently bonded;
- In the even-odd rule, an atom, as part of an ion or a molecule:
  - is represented by the letters symbolizing its name as in the periodic table,
  - has three shells: inner, inactive and covalent, each containing an even number of electrons,
  - has as many electrons in its inner shell as indicated in the periodic table,
  - has an inactive shell surrounding the inner shell and containing 0 to 4 electron-pairs,
  - has a covalent shell around the inactive shell that:
    - contains electrons that are involved in single-covalent bonds with other atoms,
    - can be empty or contain up to eight single-covalent bonds,
    - is represented in the form of lines, one line between connected atoms symbolizing a covalent bond;
- To explain the application of the rule, the letters symbolizing the element are surrounded by four information: three numbers and one signet as follow:
  - The valence number of the periodic table:
    - is indicated near the top-left corner,
    - ranges from one for elements like sodium (Na) up to eight for noble gas like Argon (Ar);
  - The charge, assigned to one atom:
    - is represented by a symbol near the top right corner,
    - uses signs + or – for a positive or negative charge respectively,
    - in the absence of charge, no symbol is used;
  - The effective-valence number:

○ is indicated near the bottom left corner,
○ is evaluated as follows: for a neutral atom *i.e.* without charge, it is equal to the valence number; for a negatively charged atom *i.e.* that possesses an extra-electron, it is the valence number increased by one; for a positively charged atom, it is the valence number decreased by one;

- The number of covalent bonds in the covalent shell:
  ○ is equal to the number of lines around the atom,
  ○ is less than or equal to the effective-valence number,
  ○ is even and starts at zero, if the effective-valence number is even,
  ○ is odd and starts at one, if the effective-valence number is odd;
- The number of electrons in the inactive shell of an atom:
  ○ is indicated near the bottom right corner,
  ○ is calculated by subtracting the effective valence-number with the number of covalent bonds,
  ○ is even; this is only possible when the number of bonds and the effective valence number are both odd or both even;
- As a consequence for the inactive shell:
  ○ It contains electron pairs that are not involved in any covalent bond,
  ○ The number of electron pairs ranges from 0 to 4 whatever the charge of the element,
  ○ When the number of electron pairs is 0, no additional covalent bond can be formed by the atom.

An important key to the validity of the even-odd rule is that the number of electrons in every shell is an even number. Specifically for the inactive shell, the even number of electrons imposes that molecules and ions belong to a group of electron-paired compounds [6] [7] *i.e.* molecules at standard energy scale [5].

In this rule, the charge translates directly into the number of electron pairs located either in the inactive shell or in the covalent shell of the atom. In the covalent shell, the charge only link to the immediate surroundings of the atom is through the covalent bonds. Its influence does not even extend to the first neighbors inactive shell. In other words, it means that a positive or negative charge is always localized on one specific atom in an ion or a molecule. It does not interfere with the compound on the whole.

In addition to the even-odd rule, an isoelectronicity rule is defined.

3. Isoelectronicity Rule

Isoelectronicity is better illustrated using two atoms like the Cl(−) ion and the Argon rare gas [9]. The number of electrons in both inactive shells and the number of covalent bonds are the same: eight and zero respectively. They are isoelectronic. They additionally both follow the even-odd rule [7].

More generally, an atom following the even-odd rule in a compound, can be replaced by another atom by using the isoelectronicity rule detailed below:

● The atom to be transformed has:
- An inner shell containing an even number of electrons,
- An inactive shell containing an even number of electrons,
- A covalent shell containing covalent bonds,
- A charge localized on the atom: negative (one added electron), positive (one removed electron) or neutral (with no local modification);

● The new atom bears similarities to the original atom:
- the same number of covalent-bonds (number of lines surrounding the atom),
- the same effective-valence number (bottom left corner of the atom),
- the same number of electrons in the inactive shell (bottom right corner of the atom);

● But its internal configuration is different:
- A different name from the periodic table,
- A different valence number,
- It meets one of the following criteria:
  ○ It belongs to the same column of the periodic table with a different inner shell.
  ○ It is the next one in the same row of the periodic table; the one-column shift is compensated by a charge to keep the effective-valence number constant (bottom left corner of the atom) and to have the same number of electrons in the inactive shell.
  ○ It is shifted in row and by column of the periodic table in agreement with both above conditions.

   ○ If the atom is charged, the sign of its charge can be reversed; in which case the replacement atom is 2 columns further in the periodic table.

Example: BH4(−) and GaH4(−) are isoelectronic compounds under the first criterion. The isoelectronicity comes from Boron and Gallium, which belong to the same column of the periodic table. As stated in the isoelectronicity rule, both atoms have the same number of covalent bonds, the same effective valence number and the same number of electrons in the inactive shell. They bear different names and don't have the same number of electrons in the inner shell.

HF and OH(−) are isoelectronic compounds under the second criterion. The isoelectronicity comes from O(−) and F, which belong to the same row and are one column apart in the periodic table. Both have one covalent-bond, an effective-valence of seven and six electrons in the inactive shell.

CH4 and PH4(+) are isoelectronic compounds under the third criterion. The isoelectronicity comes from C and P(+), which are neither in the same row of the periodic table nor in the same column. Both have 4 covalent bonds, an effective-valence number of 4 and no electron in the inactive shell.

BH4(−) and NH4(+) are isoelectronic compounds under the last criterion. B(−) and N(+) are in the same row of the periodic table and are two columns apart. Both atoms have 4 covalent bonds, an effective-valence number of 4 and no electron in the inactive shell.

4. Compounds with Elements from the Main Group of the Periodic Table

The even-odd and the isoelectronicity rules are here applied to elements of the periodic table.

Table 1 presents several atoms embedded in compounds, ions or molecules. They belong to column 1 to 8 in the main group of the periodic table: Na, Be, B, C or Si, N or P, O or S, Cl or I, Xe respectively.

Table 1. Atom of ions or molecules, in gaseous or liquid phase, compatible with the even-odd rule. Each structure represents an atom of a compound and is classified in groups having the same bottom-right number *i.e.* the same number of electrons in the inactive shell. In each group, they are ordered by increasing valence number like in the periodic table. Column one presents formulas of compounds that are composed of the atoms listed in the three other columns. Column 2 presents the positively charged element, column 3 its neutral form and column 4 its negative form. The signification of the four numbers around the letters of the element is detailed in the even-odd rule presented in chapter 2.

Number of electrons in the inactive shell = 0				
Valence number		Positive charge	neutral	Negative charge
0	--- Xe **XeCl(−)** [10]-[12]		^{0}Xe$_{0\ 0}$	^{0}Xe$^{-}_{1\ 0}$—
1	Na(+) NaF **NaF2(−)** [10] [11] [12] ..	^{1}Na$^{+}_{0\ 0}$	^{1}Na$_{1\ 0}$—	—^{1}Na$^{-}_{2\ 0}$—
2	BeH(+) BeF2 **BeF3(−)** [10] [12] [10] [11]	^{2}Be$^{+}_{1\ 0}$—	—^{2}Be$_{2\ 0}$—	—^{2}Be$^{-}_{3\ 0}$=
3	BF2(+) BH3 **BH4(−)** [10] [10] [11]	—^{3}B$^{+}_{2\ 0}$—	—^{3}B$_{3\ 0}$=	=^{3}B$^{-}_{4\ 0}$=
4	CF3(+) CH4 **SiH5(−)** [10] [10] [10]	—^{4}C$^{+}_{3\ 0}$=	=^{4}C$_{4\ 0}$=	=^{4}Si$^{-}_{5\ 0}$=
5	PH4(+) PCl5 **PCl6(−)** [10] [10] [10]	=^{5}P$^{+}_{4\ 0}$=	=^{5}P$_{5\ 0}$=	=^{5}P$^{-}_{6\ 0}$=

Continued

			Positive charge	neutral	Negative charge
6	SF5(+) [10]	SF6 [10]	SF7(−) ..	6 S + / 5 0	6 S / 6 0	6 S − / 7 0
7	ClF6(+) [10]	IF7 [10]	IF8(−) ..	7 Cl + / 6 0	7 I / 7 0	7 I − / 8 0
8	XeF7(+) [12]	Xe [12]		8 Xe + / 7 0	8 Xe / 8 0	

Number of electrons in the inactive shell = 2					
Valence number			Positive charge	neutral	Negative charge
1		Na(−)			1 Na − / 2 2
2	Be [10]	BeH(−) [10]		2 Be / 2 2	2 Be − / 3 2
3	B(+) [10]	BH [10]	BF2(−) [10]	3 B + / 2 2	3 B / 3 2	3 B − / 4 2
4	SiF(+) [10]	CH2 [12]	CF3(−) [10]	4 C + / 3 2	4 C / 4 2	4 Si − / 5 2
5	PH2(+) [11]	PCl3 [10]	PH4(−) [10]	5 P + / 4 2	5 P / 5 2	5 P − / 6 2
6	H3O(+) [10]-[12]	SeF4 [10]-[12]	SF5(−) [10]	6 S + / 5 2	6 S / 6 2	6 S − / 7 2
7	ClF4(+) [10]	IF5 [10]	IF6(−) [13]	7 Cl + / 6 2	7 I / 7 2	7 Cl − / 8 2
8	XeF5(+) [12]	XeF6 [10] [12]	XeF7(−) [12]	8 Xe + / 7 2	8 Xe / 8 2	

Number of electrons in the inactive shell = 4			
Valence number		Positive charge	neutral	Negative charge

Valence number	Positive charge	neutral	Negative charge
3				$^{3}_{4}\text{B}^{-}_{4}$
	B(−)			
4	C [10]	SiH(−) [10]		$^{4}_{4}\text{C}_{4}$	$^{4}_{5}\text{C}^{-}_{4}$
5	N(+)	N2 [8]	PH2(−) [11]	$^{5}_{4}\text{N}^{+}_{4}$	$^{5}_{5}\text{P}_{4}$	$^{5}_{6}\text{P}^{-}_{4}$
6	NO(+) [12]	H2O [10]-[12]	SeH3(−) [11]	$^{6}_{5}\text{O}^{+}_{4}$	$^{6}_{6}\text{S}_{4}$	$^{6}_{7}\text{S}^{-}_{4}$
7	ClF2(+) [10]	ClF3 [10]	ClF4(−) [10]	$^{7}_{6}\text{Cl}^{+}_{4}$	$^{7}_{7}\text{Cl}_{4}$	$^{7}_{8}\text{Cl}^{-}_{4}$
8	XeF3(+) [13]	XeF4 [10] [12]	XeF5(−) [12]	$^{8}_{7}\text{Xe}^{+}_{4}$	$^{8}_{8}\text{Xe}_{4}$	

Number of electrons in the inactive shell = 6			

Valence number	Positive charge	neutral	Negative charge
5					$^{5}_{6}\text{P}^{-}_{6}$
	P(−)			
6	O [10]-[12]	OH(−) [10]-[12]		$^{6}_{6}\text{S}_{6}$	$^{6}_{7}\text{S}^{-}_{6}$
7	**Cl(+)** [10]-[12]	HCl [10]	ClF2(−)	$^{7}_{6}\text{Cl}^{+}_{6}$	$^{7}_{7}\text{Cl}_{6}$	$^{7}_{8}\text{Cl}^{-}_{6}$
8	XeF(+) [12]	XeF2 [10]-[12]	**XeF3(−)**	$^{8}_{7}\text{Xe}^{+}_{6}$	$^{8}_{8}\text{Xe}_{6}$	

Number of electrons in the inactive shell = 8			

Valence number	Positive charge	neutral	Negative charge
7		Cl(−) [10]-[12]			$^{7}_{8}\text{Cl}^{-}_{8}$
8		Xe [10]		$^{8}_{8}\text{Xe}_{8}$	

Atoms are represented with single-covalent bonds, as if they would connect to other atoms in the compound. As defined in the even-odd rule, each atom is surrounded by one symbol, indicating the charge, and three numbers to calculate the number of electrons in the inactive shell.

In **Table 1**, atoms are grouped according to the number of electrons in the inactive shell. This even number ranges from zero to 8. Inside each group, each row corresponding to an element, is ordered by growing valence number from zero up to eight as in the periodic table. In the left column, the said valence number is indicated along with three possible compounds formulas. In the next three columns, the focus is on the element, once positively charged, once neutral and then negatively charged.

Still in **Table 1**, the number of bonds of a charged atom is deduced using the even-odd rule and the isoelectronicity rule. For example, the neutral atom in the top row is Xenon (Xe) with no bond. Adding a charge to it gives Xe(−)-right column. According to the even-odd rule, the charge is compensated with one covalent bond. In a second step, the isoelectronicity rule is applied: Xe(−) can be replace by a neutral sodium atom (Na) that is located in the middle column just below Xe. The number of bonds is maintain during the isoelectronic modification, and the neutral Na has one bond. The even-odd rule is then again used to build Na(+) without bond and Na(−) with two bonds. To build the row underneath, the isoelectronicity rule is applied to give the beryllium atom (Be). The same method alternating the even-odd and isoelectronic procedures, is used to build the other rows of **Table 1**.

In **Table 1**, the bottom right number gives the number of electrons in the inactive shell. The number is always even, implying that electrons go in pair. There cannot be more than 4 pairs in the inactive shell to ensure the coherence of the even-odd rule with the periodic table.
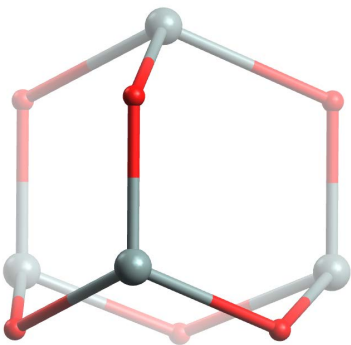
In order to show the potential of the even-odd rule, it is in the following applied to the atoms of 3D molecules.

5. The Even-Odd Rule in 3D Molecules

In previous papers, the even-odd drawing procedure has been applied to every atom of many ions or molecules [6]-[8]. In this chapter, the rule is applied to atoms in 3D molecules: two examples are displayed in **Table 2** and **Table 3**. **Table 2** relates to the P2O3 family and **Table 3** to the Si3N4 family. In the gas phase, these molecules are typically coupled [13]. The drawing software used is referenced in [14].

In the P2O3 family (**Table 2**), four molecules with numerous references in scientific literature are listed in the right column: P2O3, P2(NMe)3, (PO)2O3 and (SiR)2(PH)3 [13]. On the left side of **Table 2**, the 3D drawing of P2O3 is shown as a reference. The oxygen is symbolized in red with two bonds and the phosphorus in grey with three bonds.

Table 2. Molecules, in gaseous phase, compatible with the even-odd rule. P2O3 family.

In the middle columns, atoms composing the molecules are represented using the even-odd rule: P2O3, P2(NMe)3, (PO)2O3 and (SiR)2(PH)3. In P2(NMe)3, phosphorus P remains and the oxygen atom is replaced by NMe without charge. In (PO)2O3, the oxygen is unchanged and the phosphorus atom is replaced by PO. In this PO, the oxygen is negatively charged and the new P is positively charged to obtain a neutral molecule. In (SiR)2(PH)3, P is replaced without charge by SiR and O by the uncharged PH.

Below the 3D picture of **Table 2** is a list of 12 compounds of the P2O3 family. All of them are referenced in literature with 3D constructions [12] [13].

Table 2 illustrates clearly how the even-odd rule is an essential intermediate step between the formula and the 3D construction.

In **Table 3**, the silicon nitride family is processed in the same way. The family formula: Si3N4, is well known and serves as a reference [13]. Unfortunately, a 3D drawing of this compound is not available in literature. The author proposes a 3D representation when this molecule is coupled in a cluster: (Si3N4)2. This cluster has naturally the shape of a cube and is shown in the left column of **Table 3**: 8 nitrogen atoms in the corners and 6 silicon atoms in the face-centers. By applying the even-odd rule to the atoms of this molecule, we find that: nitrogen has 3 bonds and silicon has 4 bonds, thus giving the 3D structure.

The bonding configurations of each atom in the cluster are presented in the middle columns of **Table 3**.
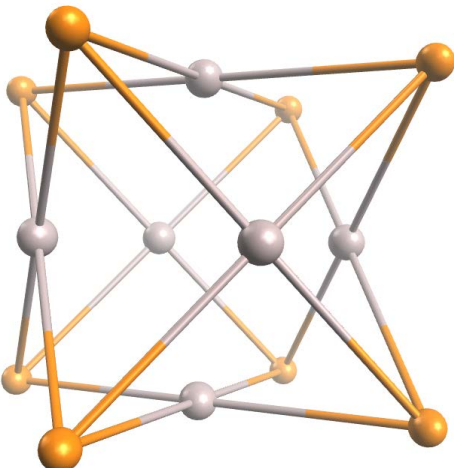
Other molecules that follow the same pattern also appear on the right side of **Table 3** [12]. Al4C3 has neutral atoms like in Si3N4. As3O4 has charged atoms and the molecules underneath are uncharged. When comparing As3O4 and As4O3, it can be seen that an oxygen atom can have 3 or 4 bonds. Both forms agree with the even-odd rule. For As3O4, the atoms are charged: half of the As atoms are positively charged and half negatively, with the same for the oxygen. By alternating the sign of charges, the overall neutrality of the molecule is guaranteed.

6. Isoelectronicity between Atoms and the Even-Odd Rule

In the present paper, the isoelectronicity rule is only applicable to single bonded compounds [8]. It also allows for an atom to be replaced by another only if no modifications occur in its interconnections. In **Table 1**, groups of three isoelectronic elements can be found by taking a diagonal going upward and to the right.

Examples of isoelectronic atoms in the second group (2 electrons in the inactive shell) are B(+), Be and Na(−). They have no bond and the same effective valence number, equal to 2. The only difference lies in the charge type. Another example with neutral carbon: N(+), C and B(−) all with 4 bonds and an empty inactive shell.

Table 3. **Molecules, in gas phase, compatible with the even-odd rule**. Si3N4 family.

3D cubic cluster with 24 bonds = 4*6			
(Si3N4)2 cluster	With 4 bonds	With 3 bonds	Molecule
	$\overset{4}{\underset{4\quad 0}{\equiv\text{Si}}}$	$\overset{5}{\underset{5\quad 2}{\equiv\text{N}}}$	(Si3N4)2 [13]
	$\overset{4}{\underset{4\quad 0}{\equiv\text{C}}}$	$\overset{3}{\underset{3\quad 0}{\equiv\text{Al}}}$	(Al4C3)2 [13]
	$\overset{5\quad +/-}{\underset{4/6\quad 0/2}{\equiv\text{As}}}$	$\overset{4\quad +/-}{\underset{3/5\quad 0/2}{\equiv\text{O}}}$	(As3O4)2 Charged [12]
	$\overset{6}{\underset{6\quad 2}{\equiv\text{O}}}$	$\overset{5}{\underset{5\quad 2}{\equiv\text{As}}}$	(As4O3)2 [12] (Sb4Sn3)2 [15] Neutral

Grey 4 bonds for: silicon, carbon, oxigen or charged arsenic
Orange 3 bonds for: nitrogen, aluminum, arsenic or charged oxigen

In the extreme positions in **Table 1**, some atoms do not belong to triplets of isoelectronic atoms. At the top are Na(+) and Xe without bond and an empty inactive shell. At the bottom, Xe and Cl(−) have no bonds and a full inactive shell. Just above, another couple Xe, Cl(−) have 3 electrons pairs in the inactive shell and two bonds. The isoelectronic candidates for these atoms are limited, exactly as the valence number in the periodic table when they are at the end of a row.

As both rules are applicable individually to each atom of a compound, the charge located on an atom does not influence the other atoms of the compound. For this reason, knowing the number of bonds an atom forms is sufficient to know the atom configuration as shown in **Table 1**.

7. Discussion

The main objective in the discussion is to compare the even-odd and the isoelectronicity rules to the classical octet and multi-bonded rules. This discussion is more general than in previous paper, which was focused on the validity of the rules [6]-[8].

7.1. The Number of Electron Pairs in the Inactive Shell and Classical Multi-Bonded Compounds

The *rule of two* for covalent bonds is classically used in molecules with single and multi-bonded atoms [2]. As a difference, the *even-odd rule* states that atoms are only bonded through single bonds. This rule also imposes that electrons go in pairs in the inactive shell. This shell has 0 electron pair, like in Na(+), up to 4 electron pairs, like in Cl(−). The difference may be interpreted as a transfer of the extra bonds in the multi bond from the covalent shell into a given number of electron pairs in the inactive shell. In the classical model, the type of bond can only be derived from the knowledge of both connected atoms whereas in the even-odd model, only one atom is needed. This different seems fundamental. Therefore, the *multi-bonds rule* and the *even-odd rule* do not have any correspondence.

7.2. The Langmuir-Octet Rule and the Empty Inactive Shell Rule

The CH_4 molecule is known as being the main representative of the octet rule [12]. Other molecules are well known, such as PH_3, H_2S and HF. In these molecules, central atoms all have 8 electrons around their inner shell (*i.e.* in the classical valence shell). This forms the fundament of the *octet rule*: atoms tend to surround themselves in the valence shell. We here would like to explore the reversed statement: what if one of the stable states of an atom in a compound is when its shell is empty? Atoms meeting this criterion are in the first group of **Table 1**. In this group, NaF, BeF_2, BH_3, CH_4, PCl_5 and SF_6 all have an empty inactive shell. Since these atoms cover every columns of the main group in the periodic table, this would seem to be an acceptable hypothesis for the *even-odd rule*. As a consequence, replacing the *octet rule* by the empty inactive shell rule seems possible. Unfortunately, this rule has a similar limitation to the *octet rule*: it is not applicable to the other groups in **Table 1**. This hypothesis to reduce the rule to about one third of possible chemical structures seems possible but too restrictive.

A better hypothesis would be to replace the *octet rule* by the *even-odd rule* including the (0 to 4) electron pairs in the inactive shell of the atoms. With this definition, this rule covers a much larger number of compounds [6]-[8], including the compounds used in **Tables 1-3**.

For example with this proposed rule, halogen can have one, three, five or seven covalent bonds without any restrictions.

7.3. Known or Unknown Compounds

Sixty-nine compounds are presented in **Table 1**. Among them, many are well documented in scientific literature: CH_4, OH(−), Na(+), H_2O, Xe and all neutral compounds. However, in the ions columns of **Table 1**, about 10% of the compounds remain unreferenced. The even-odd and isoelectronic rules help predict their existence, which has never been suggested before. They could be experimentally observed in a near future. It might also be possible that these compounds are so reactive that they rapidly form other compounds. CH_2 for instance is very unstable and rapidly reacts to form C_2H_4.

7.4. Dissociation of Diatomic Gas at High Temperature

Halogen can form diatomic molecules like for instance Cl2. By applying the even-odd rule and at high temperature, Cl2 is a gas and atoms are bonded with one bond, as mentioned in **Table 1**. Experimentally, these halogen molecules start to dissociate between 500˚C or 1000˚C-depending on the halogen [13]. Their dissociation formulas are unknown but for this dissociation, the even-odd rule proposes the existence of ions like Cl(−) and Cl(+).

These ions are important by-products of the even-odd rule and it would be very interesting to run an analysis to prove or investigate their existence.

7.5. Charge Delocalization and Charge Position

A well-known molecule like Benzene, C6H6 is classically represented with alternating single and double bonds between carbon atoms. A circle is often used to replace the double bonds, indicating that some charges are delocalized [12]. With the even-odd rule, double bonds-or the circle-must be replaced by single bonds between charged atoms, alternatively positively and negatively charged [8]. Resulting effective valence numbers of carbon atoms are either 3 or 5, depending on the atom charge, but all atoms have 3 bonds. If negatively charged, the carbon atoms have an electron pair in the inactive shell. If positively charged, the inactive shell is empty and no extra bond can be built.

As mention above with the even-odd rule, the effective valence is used to calculate the number of electron pairs near the element. The effective valence takes into account the charge of the element. A negative charge corresponds to a pair of electrons that can be located in two different shells. Either the pair is in the covalent shell, meaning an extra bond to a distinct atom or it is in the inactive shell. A positive charge corresponds to an absence of a pair also either in the covalent shell or in the inactive shell. As both shells are located near an atom, the charge is localized on a specific atom. There is no need to use the concept of delocalized electron.

This local property of the electron pairs ensures the coherence of the even-odd rule and allows us to apply the isoelectronicity rule [9].

7.6. Cubic Cluster

Page 1022 of reference [13] cites a (Me3X4)2 cluster-Me Metal and X halide–that takes a cubic form similar to that in **Table 3**. In the (Me3X4)2 cluster, atoms are in the same location as in **Table 3**. Each atom in the compound has however 8 covalent bonds unlike in **Table 3** where the cluster has 3 or 4 bonds per atom. These bonding configurations are not compatible and the isoelectronicity rule is not applicable on such a bonding configuration. A better understanding of this difference is under investigation.

7.7. Isoelectronicity Rule and Classical Multi-Bonds

Two molecules, single bonded or multi-bonded, are isoelectronic under the usual definition when they have the same total number of valence electrons [16]. In the proposed even-odd rule, compounds are single bonded and the isoelectronicity rule can be independently applied to each atom.

A classical isoelectronicity between binary compounds is mentioned by Greenwood on page 412 [13]. It lists N2, NO(+), CN(−), CO as being isoelectronic. They all have 10 valence electrons and 3 bonds. Unfortunately, the charge position is not given. If we apply the even-odd and the isoelectronicity rules described in the present paper, binary compounds must have single bonds and charges are consequently assigned to specific atoms: N2, NO(+), C(−)N and C(−)O(+). (In these four compounds, atoms are bonded through single bonds, not triple bonds like in the classical approach). All atoms have respectively an effective valence of 5 and 4 electrons in the inactive shell. From this example, we can conclude that both rules are similar except for the number of bonds. In the same way, for single-bonded compounds, classical and present isoelectronic compounds are similar: B(−)H4, CH4, N(+)H4 [9].

This similarity cannot be found for double-bonded compounds. As an example, O2, classically with a double bond has a valence number of 12. They share 4 electrons-double bond-and each oxygen atom is surrounded with 8 electrons. Classical isoelectronicity states that the diatomic compound NCl also with a double bond and 12 electrons, is an isoelectronic of O2. In the even-odd rule though, the NCl compound has one bond and both

atoms are neutral as shown in **Table 1**. Again from **Table 1**, N and Cl are isoelectronic with O(+) and O(−) respectively. As a consequence, with double bonds, compounds do not have the charges on the same atoms.

According to this last example, both isoelectronicity rules are not completely similar.

8. Conclusion

In the present article, the even-odd and the isoelectronicity rules used on chemical formulas of compounds were described. More specifically, the rules give a way to compute three numbers that are written as a convention around the name of the element. If the element is charged, the charge appears as a sign, like in classical representation. These three numbers indicate how many electron pairs are located in the three different shells of the atom. A specificity of the rules is the inactive shell, containing electrons that are available for bonding. The inactive shell only contains pairs of electrons, between 0 and 4 pairs. Another peculiarity is that both rules only deal with single-covalent bonds, indicating that multiple bonds are not needed to explain compounds configuration. More precisely, the present paper aimed to put forward both rules as a substitute to the too restrictive Langmuir-octet-rule. In order to support this claim, several atom structures from the main group in the periodic table were processed using the rules and the number of electrons pairs in the inactive shell was calculated. As presented, the structures could easily be grouped in triplets following the isoelectronic rule. As a final conclusion, the article illustrated that the even-odd and isoelectronicity rules, applied to each atom in a compound, seem to give a plausible description of single-bonded ionic or molecular structures.

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