JPII 7 (3) (2018) 333-340

Jurnal Pendidikan IPA Indonesia

http://journal.unnes.ac.id/index.php/jpii

INCOMPLETE EXPLANATION IN DETERMINING OXIDATION NUMBER: A CASE STUDY ON CHEMISTRY PROGRAM STUDENTS

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DOI: 10.15294/jpii.v7i3.13251

Accepted: February 2nd, 2018. Approved: August 31st, 2018. Published: September 20th, 2018

ABSTRACT

The term "oxidation number" and related concept such as "electronegativity" and "formal charge" appear frequently in both elementary and advance chemistry text. However, it is evident from the literature (or textbooks) that these terms are often viewed to be synonymous. Incomplete explanation of the fundamental concept of oxidation number can lead that conclusions pertaining to such a misleading interpretation. This research was conducted to review the concepts from common used high school chemistry textbooks and these concepts were then transformed to 6 number open minded problems. These problems were then tested to 40 first semester chemistry program students in the University of Jambi who joining Basic Chemistry course. The result was about 80% of students give the right answer in determining oxidation number (problem number 1). But, in the certain molecule (problem number 2) they can't determine correctly because they couldn't use the "Rule" from initial understanding in high school. For the next problem (4a), none of the students give the right oxidation number of an atom and all of them can't explain precisely correlation among oxidation number, electronegativity, and formal charge. The intent of this paper is to clarify the notion of oxidation number, electronegativity, and formal charge, describe their relationship (especially for high school chemistry textbooks), and criticize upon misleading application.

Keywords: incomplete explanation, determining oxidation number, case study, chemistry program student

INTRODUCTION

In the history of chemistry, one of the most vehement disputes concerned the nature of oxidation (Weisberg, et al. 2011; Sunarya 2009; Utami et al, 2009). In 1718, Georg Stahl, a German chemist, studied the formation of metals from oxides by heating the oxide with charcoal (carbon). He proposed that the formation of metal was caused by a substance, called "phlogiston." According to Stahl, the converse process of heating a metal in the air to form its oxide caused the release of phlogiston into the atmosphere (Sukopp, 2018). Fifty-four years later, the French chemist, Louis-Bernard Guyton de Morveau performed careful experiments showing that, during combustion, metals increase in weight. However, the existence of phlogiston was so well established among chemists that he interpreted the results as meaning that phlogiston had the negative weight (Chang, 2010; Watoni, 2016). It was his colleague, Antoine Lavoisier, who was willing to throw out the phlogiston concept and propose that combustion was due to the addition of oxygen to the metal (oxidation) and the formation of a metal from an oxide correspondent to the loss oxygen (reduction) (Stadler & Harrowfielda, 2011; Sudarmo & Sariawati 2015). This concept was well-known as "redox" concept and the most ancient concept of redox.

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Common used high school chemistry textbooks often attached development concept of redox from the ancient to the modern concept (Table 1). However, at the current time, both in elementary until advance level, the most concept has been used to explain the related concept in chemistry course is redox involved oxidation number (ON). From this concept, oxidation defines as increasing of ON, and reduction is decreasing of ON. Determining ON in high school first taught in grade X after they learn chemical bonding, atomic theory, and the periodic table of elements. Most of the commonly used chemistry text books using "the rules" approach to determine ON, without connection with the previous chapter (Österlund, et al. 2010; Permana, 2009). Besides, the fundamental concept of determining ON was much related to the previous concept.

Table 1. Redox Concept Definition from Ancient to the Modern Concept

Oxidation	Reduction
Gaining oxygen	Loosing oxygen
Loosing hydrogen	Gaining hydrogen
Loosing electron	Gaining electron
Increasing ON	Decreasing ON

Incomplete explanation of determining ON can result in misleading interpretations or misconception (Widarti et al, 2016; Harnanto & Ruminten 2009). Redox material misconception had been experienced by students (Rosenthal & Sanger, 2012; Al-Balushi et al, 2012; Setyawati, 2009) for example: they had a difficulty in distinguishing the definition of the oxygen and electrons transfer, they often experience an error in the determination of the oxidation number of atom in molecule, they did not know the key concept of oxidation and its relation to another concept i.e. electronegativity; and also they had a difficulty on how to apply the equalization to equalize the redox reactions. Misleading interpretation on determining ON will affect the students in the understanding and application of redox concept (Brandriet &Bretz, 2014; Muchtariadi, 2016; Purba 2015).

Determining ON matter in high school the first time studied in grade X after they learn chemical bonding, atomic theory, and the periodic table of element. Common high school chemistry textbook was using the "Rules" approach to determining ON. This "Rules" worked in some simple molecule, such as HCl, HNO_3, H_2SO_4, H_3PO_4, etc. But, for a more complex molecule or even simple organic molecule (ICl_5, CH_3COOH, C_2H_5OH, $Na_2S_2O_4$, $POBr_3$, H_2O_2, etc.) the "Rules" didn't work well. This phenomenon carried from high school to universities. In universities the chain of incomplete explanation of redox concept must be broken, especially through the Basic Chemistry Course. This paper aimed to give a better understanding of determining ON through complete explanation of the ON fundamental concept. Furthermore, the differences and their relation of ON concept with electronegativity, formal charge and the concept of valence were also critically discussed in this paper.

METHODS

This research employed the descriptive analysis study in the form of case study research. Forty students of Chemistry Program in the first semester (2017/2018) of University of Jambi were studied. They joined the Basic Chemistry course subject. The research instrument was an open answer test adapted from some commonly used chemistry textbook in Indonesia (Table 2). The textbook code A to E is an e-book published by Bookkeeping Center of the Ministry of National Education (Pusbuk) as Electronic School Book (ESB) which based on author's experience it is still used as a learning source for High School students. The textbook F to I is a printed textbook which very easy to find because it was available in any bookstore in Indonesia.

Six open answers problems (Table 3) and the analysis of problem choice were given in the test before entering the Redox Reaction chapter (pre-test). The answer given by the students was a reflection of their thinking ability and their understanding of the concept learned before (in high school).

Table 2. Common Used Chemistry Textbooks as a Source of Instrument Research Problems

Code	Textbook Identity
A	Setyawati, A.A. (2009). Pusbuk ESB
B	Permana, I. (2009). Pusbuk ESB
C	Sunarya, Y & Setiabudi, A. (2009) Pusbuk ESB
D	Utami, D et al., (2009). Pusbuk ESB
E	Harnanto, A. & Ruminten. (2009). pusbuk ESB
F	Sudarmo, U. & Sariwati, E. (2015). Erlangga
G	Purba. M. (2015). Erlangga
H	Muchtariadi. (2016). Yudhistira
I	Watoni, H., Kurniawati, D., & Juniastri, M. (2016). Yrama Widya

RESULTS AND DISCUSSION

Determining the Oxidation Number

As stated before, common used high school chemistry textbooks use the “Rules” for determining ON. Here is a summary of these “Rules” from common used high school chemistry textbooks:

(1) ON of free atom is zero;
(2) Sum of ON in a neutral atom is zero;
(3) ON of monoatomic ion is equal to its charge;
(4) Sum of ON in a polyatomic ion is equal to its charge;
(5) ON of oxygen atom generally is -2, but it is -1 in peroxide, and -1/2 in superoxide;
(6) ON of hydrogen atom generally is +1, but it is +1 in hydride;
(7) ON of another atom, determined from its group, such as group IA generally is +1, IIA is +2, IIIA is +3, VIIA generally is -1 etc.

It is mention in these textbooks some example of an atom in a molecule that the ON would be determined: “Determine the ON of S (sulfur) atom in H_2SO_4!”. Using rule number (2), (5), and (6), the calculation can be express:

(2×ON of H) + (1× ON of S) + (4×ON of O) = 0
(2×+1) + (ON of S) + (4×-2) = 0
(+2) + ON of S + (-8) = 0
ON of S = +6

The other example that can be solved using the “rules” were $K\underline{Mn}O_4$, $Na\underline{Cl}$, $K_2\underline{Cr}_2O_7$, $H\underline{N}O_3$, $H_3\underline{P}O_4$, $\underline{S}O_3$, $\underline{Fe}_2O_3$, $\underline{V}_2O_5$, etc. (the underlined atom was atom will be determined its ON).

Table 3. The Problems Summary Adapted from Common Used High School Chemistry Textbooks

Num.	Problem	Analysis
1	Determine the oxidation number of each atom in the molecule below! a. HNO_3 b. Fe_2O_3 c. $KMnO_4$ d. $K_2Cr_2O_7$ H : Fe : K : K : N : O : Mn : Cr : O : O : O :	C3 Level. ON of each atom of this molecule can be easily determined by “The Rules”.
2	Determine the oxidation number of each atom in the molecule below! a. KO_2 b. NaH c. H_2O_2 d. OF_2 K : Na : H : O : O : H : O : F :	C3 Level. “The Rules” still partly applied, but the student starts to confuse especially to determine the sign (+) or (-).
3	Based on what theory you choose each oxidation number in problem number 2?	C4 Level. The students should explain based on what thy choose (+) or (-) sign in ON.
4	Determine the oxidation number of each atom in the molecule below! a. $S_3O_2^{2-}$ b. $POBr_3$ c. CH_3COOH d. ICl_5 S : P : C : I : O : O : H : Cl : Br : O :	C4 Level. “The Rules” completely can’t be used. ON determined by Lewis structure interpretation and electronegativity concept.
5	Based on what theory you choose each oxidation number in problem number 4?	C4 Level. The students should explain based on what thy choose (+) or (-) sign in ON.
6	Determine the formal charge for each atom in problem number 4! Can you explain the nature of formal charge compares with oxidation number? S : P : C : I : O : O : H : Cl : Br : O :	C4 Level. Formal Charge is “ownership” of an electron if shared evenly. In high school FC has almost never been introduced.

The results of problem 1 appear in Figure 1. These results indicated the good understanding of some molecule that its ON can be solved by the "Rules". The wrong answers were caused by mistake assumption that ON belongs to a group of the atom. The right concept was ON belongs to only a single atom. The percentage of the right answers to problem 1 can be seen in Figure 1.

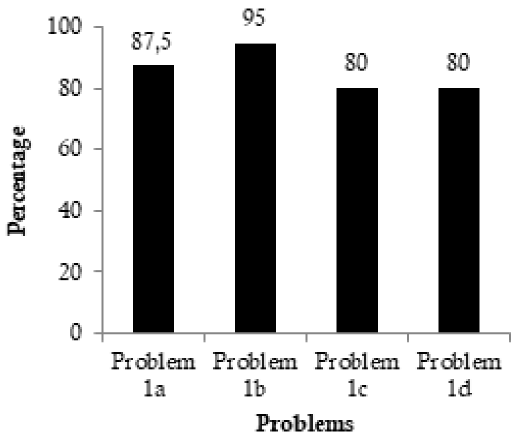


Figure 1. The Right Answers Percentage of Problem 1

Overall, the right answers percentage above 80%, so problem 1 successfully solved using "The Rules".

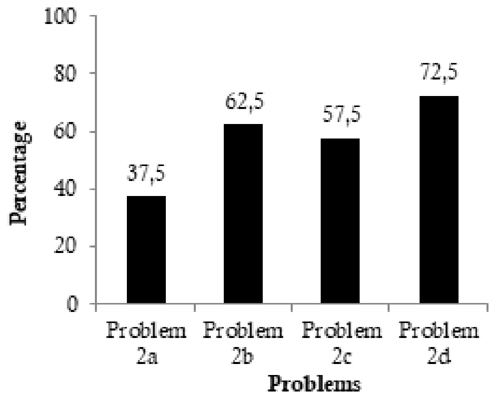


Figure 2. The Right Answers Percentage of Problem 2

The Correlation of ON, Chemical Bonding, and Electronegativity

The problems emerged when the students try to solve Problem 2. They were confused determined ON of each atom especially its sign, (+) or (-). Even tough, almost 50% give the right answers, but them just guessing. They haven't a fundamental concept to confirm their results. This proven by them that they can't answer Problem 3. Some students answer "Exceptional", but still, they didn't know for sure when using "exceptional" and "common" one.

Table 4. Electronegativity of Pauling Scale Several Selected Atoms (Mann, et al. 2000)

1	2	12	13	14	15	16	17	18
H 2.300								He 4.160
Li 0.912	Be 1.576		B 2.051	C 2.554	N 3.066	O 3.610	F 4.193	Ne 4.787
Na 0.869	Mg 1.293		Al 1.613	Si 1.916	P 2.253	S 2.589	Cl 2.689	Ar 3.242
K 0.734	Ca 1.034	Zn 1.588	Ga 1.756	Ge 1.994	As 2.211	Se 2.424	Br 2.685	Kr 2.966
Rb 0.706	Sr 0.963	Cd 1.521	In 1.656	Sn 1.824	Sb 1.984	Te 2.158	I 2.359	Xe 2.582
Cs 0.659	Ba 0.881	Hg 1.765	Tl 1.789	Pb 1.854	Bi (2.01)	Po (2.19)	At (2.39)	Rn (2.60)

Problem 2 shows us that ON is very related to another concept. The concepts that so related with ON were electronegativity and chemical bonding. The definition by its terminology of ON is the charge remaining on an atom when all ligands are removed heterolytically in their closed form, with the electron being transferred to the more electronegative partners; homonuclear bonds do not contribute to the ON (Parkin, G., 2006). Table 4. shows the value of electronegativity by Pauling scale on several selected atom (Jensen, 2012; Chattaraj & Duley, 2010).

From the explanation of redox definition above, it can conclude two things; first, ON can be determined from differences between electronegativity values. It was because the differences in electronegativity values lead to the type of chemical bonds. If the differences were great, the substance tends to ionic, otherwise if slight, it tends to covalent. The level of ionic character can be determined by calculation of moment dipole (Miessler et. al., 2014) and covalent character can be determined by Fajans Rule i.e. calculation of charge density/polarization of molecule (Canham & Overton, 2010). Based on both methods, there is no molecule with 100% of ionic/covalent character. The term ionic/covalent compound means it has greater ionic/covalent, not pure ionic/covalent compound (Wells, 2012; Diercks & Yaghi, 2017).

The second, ON concept is designated for a substance that has wide electronegative differences, thus, the substance assumed tend to ionic. These electronegative differences cause the heterolytic cleavage, where the electron will give to the atom with greater electronegativity. If the atom in substance has the same electronegativity, so the substance tends to covalent and cause the homolityc cleavage, where the electron will be share equally to each atom/ligands. This condition obtains a new unit called a formal charge (FC). The calculation of ON and FC can be seen below (Figure 3).

ON = Number of electrons in valence shell of free atom. → Number electrons remaining on atom in molecule after all bonds are broken heterolytically.

FC = Number of electrons in valence shell of free atom. → Number of electrons remaining on atom in molecule after all bonds are broken homolytically.

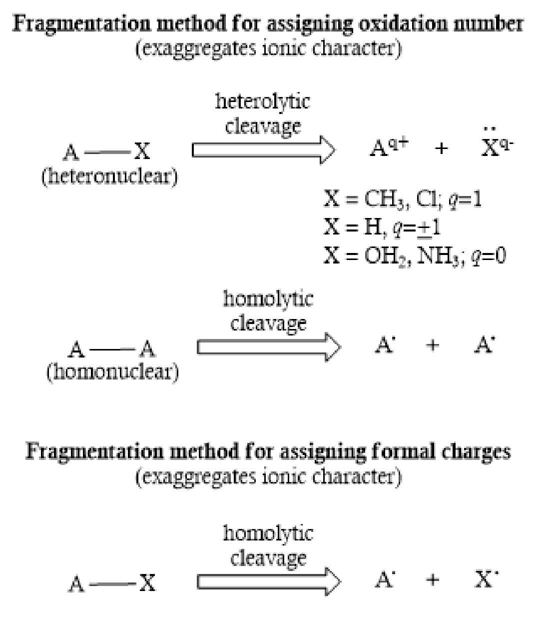


Figure 3. Fragmentation Methods for Assigning the Oxidation Number and the Formal Charge.

Determining ON based on this concept requires drawing the Lewis structure (electron-dot) that molecule. Whereas, an electron in covalent polar bond is not fully shared together, to simplify the ON calculation it is assumed that electron "belong to" atom with greater electronegativity. Example of determining some common compound can be seen in Figure 4.

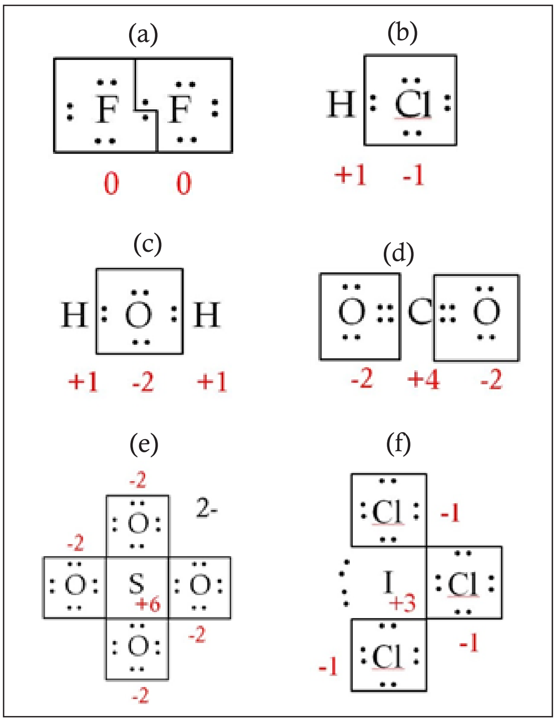


Figure 4. Determining ON of Some Common Compounds by Heterolytic Cleavage

Figure 4(a) explains why the free molecule has ON zero. Fluorine atom in the F_2 molecule has the same electronegativity, so will be a homolitycal cleavage, where electron shared equally. So, ON of both F atom can be count as 7 – 7 = 0. The same principle can be applied to Figure 4 (b) to (f) that electron as if "belong to" the more electronegative atom. Then, the right answer of problem number 3 and 5 was "electronegativity". Only 15% (6 students) give the right answer, the rest of them reply with "because of the rule" answers.

From the explanation presented in Figure 4, we can determine ON compound in problem 4 correctly (Figure 5). The bond symbolized by line (–) means the pairs of the electron. The right answers percentage of Problem 4 shows in Figure 6. The entire students think that ON of sulfur atom in $S_2O_3^{2-}$ ion (Figure 5a) has the same value, +2. Using "The Rules" they count 2× (ON S) + 2×(-2) = -2. This calculation can't be accepted because each of sulfur has a different environment.

ON of S (center) has only 1 electron left because it is bonding with 3 oxygen atoms which have a higher electronegativity than S and 1 S atom which have equal electronegativity. So, calculation can be written ON S (center) = 6 – 1 = +5, for S (side) ON = 6 – 7 = -1. Calculation of FC (Problem 6) cannot be answered correctly by all students. The FC sound so strange in students because FC concept was not introduced in high school (Loock, 2010). All students confirm that there is no explanation about FC in the previous place (high school or university). In high school (or university) FC can be taught related to VSEPR topics (Taber, 2013).

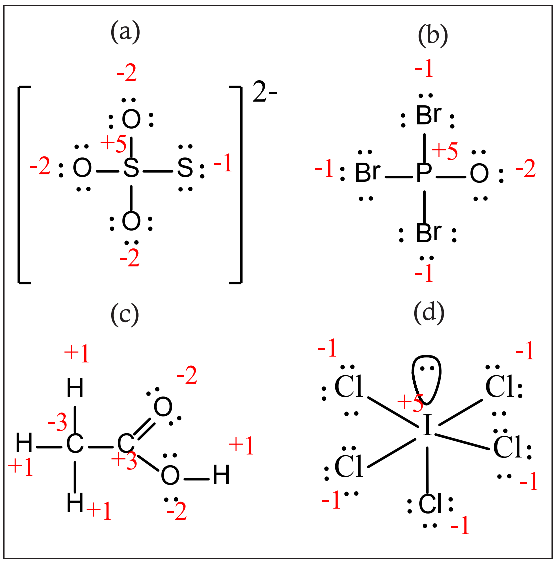


Figure 5. The ON of an Atom in the Molecule at Problem 4

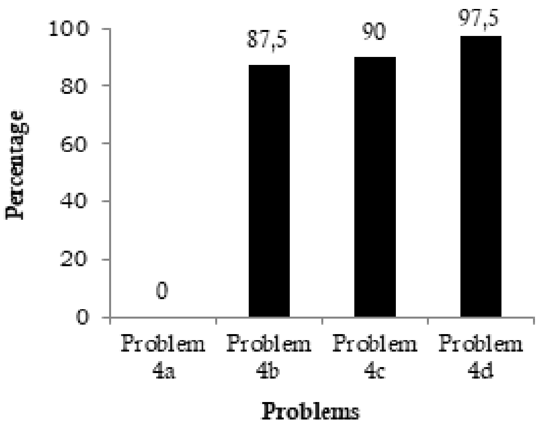
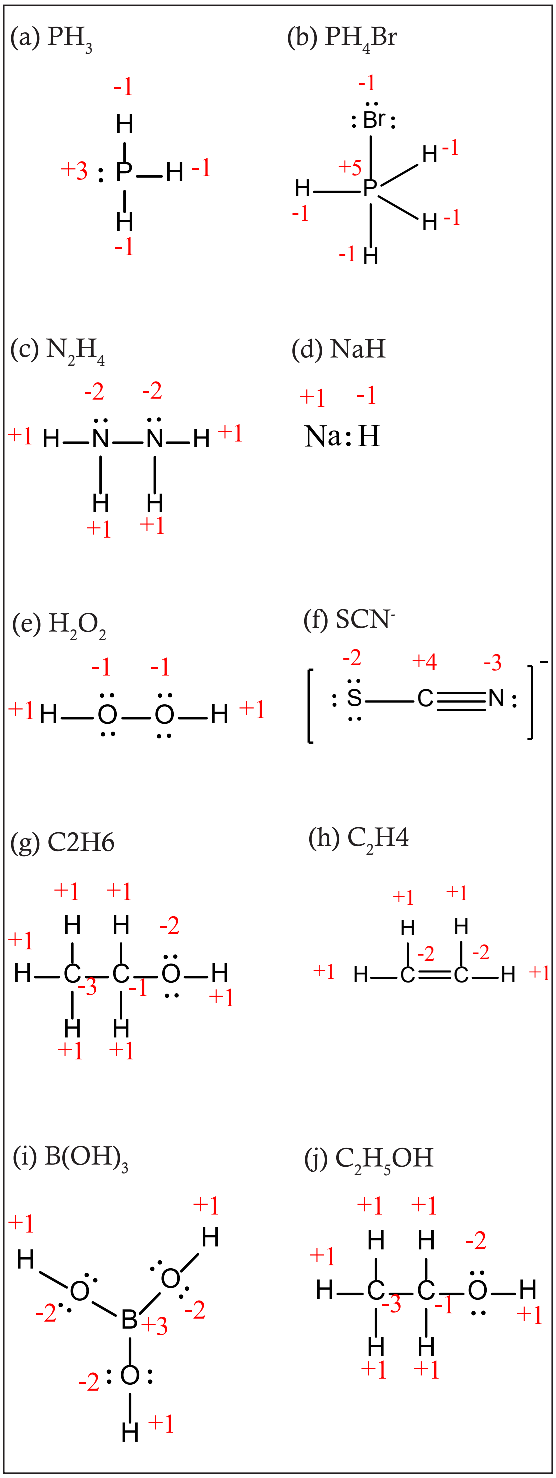


Figure 6. Right Answers Percentage of Problem 4

Memorizing "The Rules" for determining ON was not so helpful if the deal with the more complex compound. Some compound only can be determined the ON by the combination of Lewis structure and electronegativity. Using "the rules" to determine ON of complex compound can lead to mistake knowledge and misconception (Regan et al, 2011). From 9 common high school chemistry textbooks (Table 2), only 2 books provide the information of electronegativity to determine ON. However there was still had some mistakes in the example. Here is some common compound in some textbook which often mistakes in determining of ON (Figure 7).



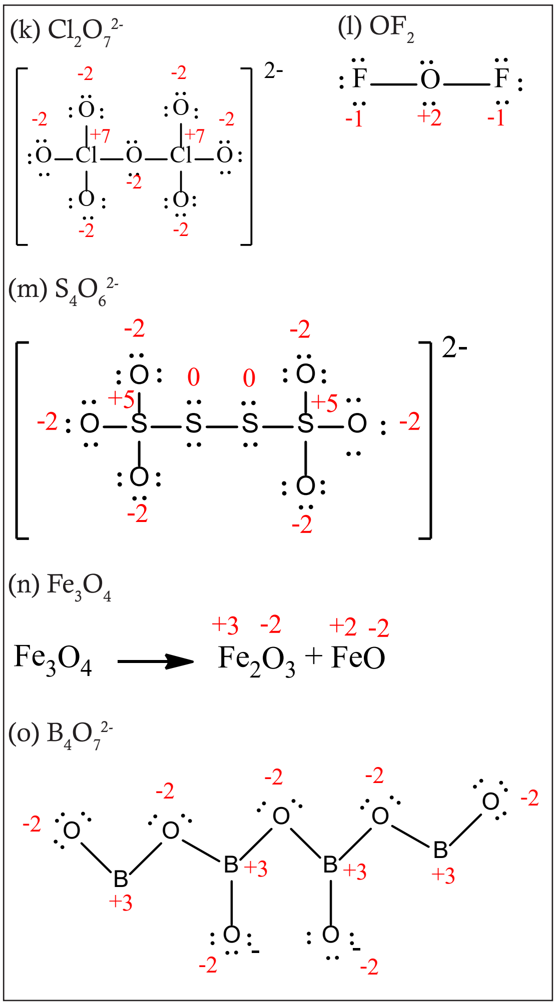


Figure 7. The Common Compound which often Mistakes in Determining the ON

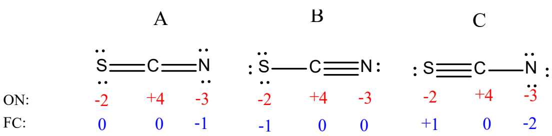


Figure 8. ON and FC of Thiocyanate Ion Resonance

The difference of the fundamental approach between ON and FC has important consequences: ON is independent; it is not depending on molecular structure (Lewis Structure). But, FC is changed depending from its Lewis structure. The Example of this phenomenon can be seen in thiocyanate ion resonance (Figure 8).

CONCLUSION

ON is an important concept in both elementary and advance chemistry. Learning ON in high school or in the beginning year in the university should be taught by the related concept: electronegativity and Lewis structure. This case study research concludes that the most of the students only know "The Rules" as initial knowledge from High School to determining oxidation number. These leads most of the students can solve Problem No. 1 and No. 2 which was simple molecules that can be solved using "The Rules". For the next problem (No.3 – No.6), less than 10% students give the correct oxidation number of an atom and none of them can explain precisely correlation among oxidation number, electronegativity, and formal charge. Learning ON in High School (or in the beginning year in university) should be taught by the related concept: electronegativity and Lewis structure supported by chemistry text book containing complete related concept. Without learning these connection concepts, misconceptions tend to occur and the student will struggle to learn chemistry.

ACKNOWLEDGEMENTS

The author(s) thanks Prof. Sutrisno, Ph.D as former dean of the Faculty of Science and Technology, Universitas Jambi for facilitating this work.

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