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Using the Carbon-Atom Method to Determine Mean Oxidation Number of Organic Carbons

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Abstract

The notion of oxidation number acting as an electron-counting concept is crucial for balancing redox reactions, and for understanding organic and biological redox conversions. Chemical formula methods are widely used for counting oxidation numbers. There are three types of chemical formula methods. They are molecular formula method, structural formula method, and Lewis formula method. Each type has its own rules and procedures, and they are difficult for students to fully understand and remember. In addition, the capability of the molecular formula method to assign mean oxidation number of organic carbons for organic molecules or molecular ions is limited. To overcome these drawbacks, this article explores a new half reaction approach, the carbon-atom method, which can count the mean oxidation number of organic carbons for both organic and bioorganic compounds. The quantitative relationships among the number of transferred electrons, change in oxidation numbers of organic carbons, and mean oxidation number of organic carbons can also be established by balancing half organic reactions. Furthermore, the mean oxidation number of organic carbons for any given organic or bioorganic compounds with known structural formulas can be determined by using the carbon-atom method and the fragmentation operation.

Keywords: carbon-atom method, balancing half redox equation, number of transferred electrons, change in oxidation numbers, mean oxidation number of organic carbons, fragmentation operation, organic fragmentated $C_xH_yO_z^{charge}$

1. Introduction

Redox reaction is of central importance in chemistry and biochemistry (Goodstein, 1970; Ochs, 2019). It is an electron-transfer reaction, which is composed of the oxidation and reduction of two half reactions. It can also be understood as the increase and decrease of the oxidation number of atoms (ON) (IUPAC, 2019). Chemical formula methods are used for determining ON. There are three types, namely, molecular formula method, structural formula method, and Lewis formula method (Kauffman, 1986; Halkides, 2000; Bentley, Franzen & Chasteen, 2002; Menzek, 2002; Loock, 2011; Jurowski, Krzeczkowska & Jurowska, 2015; Yuen & Lau, 2022a). They are all substance-based methods. Each type has its own rules and procedures, and it is difficult for students to fully understand them. Among the three types, the molecular formula method is widely used for defining and balancing redox reactions at the level of general chemistry. However, when there is a lack of structural information, it may not be possible to assign mean oxidation number of organic carbons (ONc) for organic molecules or molecular ions.

On the other hand, although the oxidation number of organic carbon is used as an analytical tool to facilitate the understanding of redox pathways in metabolism (Hanson, 1990; Halkides, 2000; Bentley, Franzen & Chasteen, 2002), the concept was not mentioned in some organic chemistry or biochemistry textbooks. Even in books where the concept can be found, the relationship between the mean oxidation number of organic carbons (ONc) and the number of transferred electrons (Te^-) was not established (Robert & Caserio, 1977; Soderberg, 2019).

The most convenient balancing method that is found in textbooks and research journals (Tro, 2020; Chang & Goldsby, 2013; Kolb, 1978; Generalic & Vladislavic, 2018) is the ion-electron method, which is a half reaction method based on ON counting. It has four sequential steps: (i) assign all ON before and after redox reactions; (ii) count change in oxidation numbers (ΔON); (iii) calculate Te^-; and (iv) equalize Te^- of two half reactions. However, when ON cannot be assigned, this method is not applicable. Consequently, the learning of redox reactions will be adversely affected (Garnett & Treagust, 1992; De Jong, Acampo & Verdonk, 1995; Brandriet & Bretz, 2014).

The mathematical relationships between Te^- and ΔONc (Yuen & Lau, 2022b), and that among net-charge, Te^-, and ΔONc (Yuen & Lau, 2023) have already been formulated. This article explores a new approach, the carbon-atom (C-atom) method, which can establish the relationships among Te^-, change in mean oxidation numbers of organic carbons (ΔONc), and ONc. It can also count ONc for both organic and bioorganic compounds by using the fragmentation operation. It is a reversed ion-electron method, the sequence of which begins with balancing a half reaction, counting Te^-, calculating ΔONc, and then assigning ONc. The C-atom method can overcome the limitations of the ion-electron method and is beneficial for the teaching and learning of organic redox reactions. Step-by-step procedures and examples will be demonstrated in the following sections.

2. Mean ONc and Individual ONc

The molecular formula method can only be used for counting the mean ONc whereas the structural formula method can be used for counting both the mean ONc and individual ONc (Yuen & Lau, 2022a). Characteristics of the molecular formula method and the structural formula method for organic compounds are compared in Table 1. Examples for counting mean ONc and individual ONc are provided as follows.

Table 1. Characteristics of molecular formula method and structural formula method

Method	Molecular formula method	Structural formula method
Requirement	a molecular formula	a structural formula
Operation	rules and assumptions	fragmentation, the difference in electronegativity (Δχ) between two atoms forming covalent bond(s)
Counting	mean ONc	individual ONc and mean ONc
Mathematical equation	$\Sigma ON_i = 0$ (for neutral particles) $\Sigma ON_i \neq 0$ (for charged particles)	mean ONc = $\frac{\Sigma \text{ individual ONc}}{\text{nc}}$

An organic chemical formula of $C_2H_6S_2$ containing undefined mean oxidation number of sulfur (ON_S) is provided as an example here. Regarding the mathematical equation $2ONc+6ON_H+2ON_S = 0$ ($ON_H = +1$), an assumed value of ON_S is needed to count ONc. Different assumed values of ON_S will produce different results of ONc. Regarding the molecular formula $C_2H_6S_2$, the shown structural formulas of CH_3-S-S-CH_3, HS-CH_2-CH_2-SH, and CH_3-S-CH_2-SH are its isomers. Based on their identified structural formulas, all individual ON_H, ONs, and ONc can be assigned accordingly.

2.1 Examples: Counting Mean ONc by Using Molecular Formula Method

Example 1a. Given C_2H_4O	Example 1b. Given C_2H_6O
Solve: by using $\Sigma ON_i = 0$	Solve: by using $\Sigma ON_i = 0$
$2ONc+4ON_H+1ON_O = 0$	$2ONc+6ON_H+1ON_O = 0$
ONc = $\frac{-4\,ON_H - 1\,ON_O}{2}$	ONc = $\frac{-6\,ON_H - 1\,ON_O}{2}$
∵ $ON_H = +1$; $ON_O = -2$	∵ $ON_H = +1$; $ON_O = -2$
∴ mean ONc (C_2H_4O) = $\frac{-4(+1)-1(-2)}{2}$ = -1	∴ mean ONc (C_2H_6O) = $\frac{-6(+1)-1(-2)}{2}$ = -2

2.2 Examples: Counting Individual ONc and Mean ONc by Using Structural Formula Method

Example 2a. Given CH_3CHO	Example 2b. Given CH_3CH_2OH
Solve: by using fragmentation operation	Solve: by using fragmentation operation
Fragments: CH_3, CHO	Fragments: CH_3, CH_2^+, ^-OH
individual ONc = -3, +1	individual ONc = -3, -1
by using mean ONc = $\frac{\Sigma \text{ individual ONc}}{\text{nc}}$	by using mean ONc = $\frac{\Sigma \text{ individual ONc}}{\text{nc}}$
mean ONc = $\frac{(-3)+(+1)}{2}$= -1	mean ONc = $\frac{(-3)+(-1)}{2}$= -2

2.3 Defining the Redox Nature by Using Individual ONc and Mean ONc

According to the IUPAC rule (IUPAC, 2019), an increase of ON corresponds to oxidation whereas a decrease of ON corresponds to reduction. The concepts of individual ONc and mean ONc are applied to define each individual carbon redox site and half redox reaction respectively.

Example 3. Given $CH_3CHO \longrightarrow CH_3CH_2OH$

Solve:

Conversion	CH_3CHO	⟶	CH_3CH_2OH
individual ONc	-3; +1		-3; -1
mean ONc	-1		-2

In example 3, there is no change in individual ONc from CH_3 (-3) to CH_3 (-3). It represents a non-redox carbon atom site. There is a decrease of individual ONc from CHO (+1) to CH_2OH (-1). It represents a reduction carbon atom site. Also, a decrease of mean ONc = -1 (CH_3CHO) to mean ONc = -2 (CH_3CH_2OH) is shown. Therefore, the conversion of "$CH_3CHO \longrightarrow CH_3CH_2OH$" is defined as a half reduction reaction.

3. Determining the Change in Mean Oxidation Numbers of Organic Carbons (∆ONc)

Regarding a redox couple, the relationships among Te^-, n_{atom}, and ΔON_{atom} in a balanced half reaction have already been established (Yuen & Lau, 2022b). It is shown and used here as $Te^- = nc \times \Delta ONc$. Either Te^- or ∆ONc can be used as a redox criterium for defining organic half reactions (shown in Table 2).

Table 2. Te^- or ∆ONc as a redox criterium for defining organic half reactions

Half redox reaction	Number of transferred electrons			Change in mean oxidation numbers of organic carbons		
oxidation	loss of e^-	$Te^- > 0$	(+)	increase	$\Delta ONc > 0$	(+)
reduction	gain of e^-	$Te^- < 0$	(-)	decrease	$\Delta ONc < 0$	(-)
non-redox	no gain or loss of e^-	$Te^- = 0$	0	no change	$\Delta ONc = 0$	0

∆ONc can be determined by the following equations:

$$\Delta ONc = \frac{Te^-}{nc}$$

∆ONc = change in mean oxidation numbers of organic carbons

Te^- = number of transferred electrons

nc = number of organic carbons

∆ONc = ONc (product) - ONc (reactant)

ONc (product) = mean oxidation number of organic carbons of the product

ONc (reactant) = mean oxidation number of organic carbons of the reactant

The method is shown in the scheme below and demonstrated in Example 4:

balancing a half reaction ⟶ counting Te^- and nc ⟶ calculating ∆ONc

Example 4. Conversion of acetaldehyde to ethanol

Solution: acetaldehyde ⟶ ethanol

$CH_3CHO \longrightarrow CH_3CH_2OH$

$C_2H_4O \longrightarrow C_2H_6O$

$C_2H_4O + 2H^+ \longrightarrow C_2H_6O$

$C_2H_4O + 2H^+ + 2e^- \longrightarrow C_2H_6O$

$Te^- = -2$; nc = 2

∆ONc = ONc (CH_3CH_2OH) - ONc (CH_3CHO)

$$\Delta ONc = \frac{Te^-}{nc}$$

$$= \frac{(-2)}{2}$$

$$= -1$$

With reference to Table 2, in the half reaction of "$C_2H_4O + 2H^+ + 2e^- \longrightarrow C_2H_6O$", 2 carbon atoms (nc) gaining 2 electrons (Te^-) represents mean ΔONc equals -1. The value of mean ΔONc is less than zero (< 0), therefore, it is a reduction reaction.

4. Determining the Mean Oxidation Number of Organic Carbons (ONc) for Organic Compounds

The established mathematical equations in balanced half reactions are shown below:

$$Te^- = nc \times \Delta ONc$$

$$\Delta ONc = ONc\ (product) - ONc\ (reactant)$$

$$ONc\ (reactant) = ONc\ (product) - \frac{Te^-}{nc}$$

If ONc (product) is known, then ONc (reactant) can be derived and counted accordingly.

$$ONc\ (unknown) = ONc\ (known) - \frac{Te^-}{nc}$$

The known oxidation number of carbon (ONc) for a carbon-atom (C) equals 0. By letting C be a designated known product in an organic half reaction, the mean ONc of an organic molecule or molecular ions can be calculated effectively. By converting the molecules or molecular ions to C in half equations, their mathematic equations for the unknown mean ONc are shown below:

organic molecule/molecular ion ⟶ C

$$mean\ ONc\ (organic\ molecule/molecular\ ion) = ONc\ (C) - \frac{Te^-}{nc}$$

$$= 0 - \frac{Te^-}{nc}$$

$$= -\frac{Te^-}{nc}$$

In the following operating procedures, C is chosen as the designated product of a half reaction. An unknown mean ONc of organic molecules or molecular ions can be calculated by Te^- and nc accordingly.

5. C-atom Method for ONc: Procedures and Examples

The C-atom method is a half reaction-based method, which can count ONc by converting a molecular/ionic organic particle to C-atom in a half reaction. It is demonstrated in the scheme below:

balancing half reactions ⟶ counting Te^- and nc ⟶ calculating ONc

When using the balancing half reaction method, H^+, O, H_2O, and electron (e^-) are employed as devices (Yuen & Lau, 2022b). The operating procedures for an organic fragmentated $C_xH_yO_z^{charge}$ (molecule, charge = 0; molecular ion, charge ≠ 0) in Examples 5 to 7 are shown below:

Step 1. Balance atoms
- 1.1 balance carbon atoms
- 1.2 balance each O atom by adding one O
- 1.3 balance each H atom by adding one H^+
- 1.4 convert each extra O atom to one H_2O by adding two H^+

Step 2. Add electrons to make charges equivalent

Step 3. Count Te^- and nc

Step 4. Calculate ONc

Example 5. Determine the mean ONc of CH_3CH_2OH

Solution: $C_2H_6O \longrightarrow C$

$C_2H_6O \longrightarrow 2C$

$C_2H_6O \longrightarrow 2C + 6H^+ + O$

$C_2H_6O + 2H^+ \longrightarrow 2C + 6H^+ + O + 2H^+$

$C_2H_6O \longrightarrow 2C + H_2O + 4H^+$

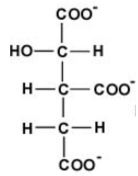
$C_2H_6O \longrightarrow 2C + H_2O + 4H^+ + 4e^-$

$Te^- = +4$; nc = 2

$$ONc\ (CH_3CH_2OH) = -\ \frac{Te^-}{nc}$$

$$= -\ \frac{(+4)}{2}$$

$$= -2$$



Example 6. Determine the mean ONc of isocitrate,

Solution: $C_6H_5O_7^{-3} \longrightarrow C$

$C_6H_5O_7^{-3} \longrightarrow 6C + 7O + 5H^+$

$C_6H_5O_7^{-3} + 14H^+ \longrightarrow 6C + 7O + 5H^+ + 14H^+$

$C_6H_5O_7^{-3} + 9H^+ \longrightarrow 6C + 7H_2O$

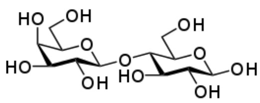
$C_6H_5O_7^{-3} + 9H^+ + 6e^- \longrightarrow 6C + 7H_2O$

$Te^- = -6$; nc = 6

$$ONc\ (C_6H_5O_7^{-3}) = -\ \frac{Te^-}{nc}$$

$$= -\ \frac{(-6)}{6}$$

$$= +1$$



Example 7. Determine the mean ONc of lactose,

Solution: $C_{12}H_{22}O_{11} \longrightarrow C$

$C_{12}H_{22}O_{11} \longrightarrow 12C + 11O + 22H^+$

$C_{12}H_{22}O_{11} \longrightarrow 12C + 11O + 22H^+$

$C_{12}H_{22}O_{11} \longrightarrow 12C + 11H_2O$

$Te^- = 0$; nc = 12

$$ONc\ (C_{12}H_{22}O_{11}) = -\ \frac{Te^-}{nc}$$

$$= -\ \frac{(0)}{12}$$

$$= 0$$

6. Assigning ONc for Organic and Bioorganic Compounds

Organic and bioorganic compounds are mainly composed of seven types of elements, which are carbon (C), hydrogen (H), oxygen (O), halogen (X), nitrogen (N), sulfur (S), and phosphorous (P). They are represented by the general chemical formula $C_xH_yO_zX_wN_vS_uP_t$. In cases where carbon-peroxide, carbon-heteroatom, or carbon-oxygen-heteroatom bond is present in organic compounds, the fragmentation operation is needed prior to counting ONc (Yuen & Lau, 2022a; 2022c). First, these molecules are divided into two or more organic and inorganic fragments; second, all organic fragments are summarized by their individual organic chemical formulas; and third, ONc can be counted by the summarized organic chemical formula as an organic fragmentated $C_xH_yO_z^{charge}$. The procedures are shown in the following examples.

Example 8. Determine the mean ONc of $CH_3OOCH_2CH_3$

Solution: Breaking carbon-peroxide bonds

$CH_3OOCH_2CH_3 \longrightarrow CH_3^+$ (organic fragment) + $^-OO^-$ (inorganic fragment) + $^+CH_2CH_3$ (organic fragment)

$CH_3OOCH_2CH_3 \longrightarrow C_3H_8^{2+}$ (summarized organic fragments) + $^-OO^-$

$C_3H_8^{2+} \longrightarrow C$

$C_3H_8^{2+} \longrightarrow 3C + 8H^+$

$C_3H_8^{2+} \longrightarrow 3C + 8H^+ + 6e^-$

$Te^- = +6$; $nc = 3$

$$ONc\ (C_3H_8^{2+} \text{ or } CH_3OOCH_2CH_3) = -\frac{Te^-}{nc} = -\frac{(+6)}{3} = -2$$

Example 9. Determine the mean ONc of $CH_3C(O)CH_2S(O)_2CH_3$

Solution: Breaking carbon-sulfur bonds

$CH_3C(O)CH_2S(O)_2CH_3 \longrightarrow CH_3C(O)CH_2^+$ (organic fragment) + $^-SO_2^-$ (inorganic fragment) + $^+CH_3$ (organic fragment)

$CH_3C(O)CH_2S(O)_2CH_3 \longrightarrow C_4H_8O^{2+}$ (summarized organic fragments) + SO_2^{-2}

$C_4H_8O^{2+} \longrightarrow C$

$C_4H_8O^{2+} \longrightarrow 4C + 8H^+ + O$

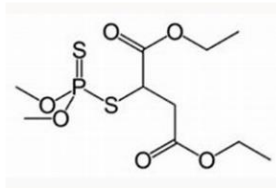
$C_4H_8O^{2+} + 2H^+ \longrightarrow 4C + 8H^+ + O + 2H^+$

$C_4H_8O^{2+} \longrightarrow 4C + 6H^+ + H_2O$

$C_4H_8O^{2+} \longrightarrow 4C + 6H^+ + H_2O + 4e^-$

$Te^- = +4$; $nc = 4$

$$ONc\ (C_4H_8O^{2+} \text{ or } CH_3C(O)CH_2S(O)_2CH_3) = -\frac{Te^-}{nc} = -\frac{(+4)}{4} = -1$$

Example 10. Determine the mean ONc of Malathion, , $C_{10}H_{19}O_6S_2P$

Solution: Breaking carbon-oxygen (from carbon-oxygen-heteroatom) bonds and carbon-sulfur bond

$C_{10}H_{19}O_6S_2P \longrightarrow 2CH_3^+$ (organic fragment) + $^{-2}O_2PSS^{-1}$ (inorganic fragment) + $^{+}C_8H_{13}O_4$ (organic fragment)

$C_{10}H_{19}O_6S_2P \longrightarrow C_{10}H_{19}O_4^{3+}$ (summarized organic fragments) + $O_2PS_2^{-3}$

$C_{10}H_{19}O_4^{3+} \longrightarrow C$

$C_{10}H_{19}O_4^{3+} \longrightarrow 10C + 19H^+ + 4O$

$C_{10}H_{19}O_4^{3+} \longrightarrow 10C + 19H^+ + 4O$

$C_{10}H_{19}O_4^{3+} + 8H^+ \longrightarrow 10C + 19H^+ + 4O + 8H^+$

$C_{10}H_{19}O_4^{3+} \longrightarrow 10C + 11H^+ + 4H_2O$

$C_{10}H_{19}O_4^{3+} \longrightarrow 10C + 11H^+ + 4H_2O + 8e^-$

$Te^- = +8$; nc = 10

$$\text{ONc } (C_{10}H_{19}O_4^{3+} \text{ or Malathion}) = -\frac{Te^-}{nc}$$

$$= -\frac{(+8)}{10}$$

$$= -\frac{4}{5}$$

7. Te$^-$, ΔONc, and ONc for Understanding Conversions of Organic Compounds

Quantified Te$^-$, nc, ONc, and ΔONc from Examples 4 to 10 are summarized in Table 3. By using the half reaction method, ONc, Te$^-$, or ΔONc can be used as a criterium to define organic and bioorganic conversions.

Table 3. Quantified Te$^-$, nc, ONc, and ΔONc in half reactions

Half reaction	Te$^-$	nc	ONc (Reactant)	ONc (Product)	ΔONc
$C_2H_4O + 2H^+ + 2e^- \longrightarrow C_2H_6O$	-2	2	-1	-2	-1
$C_2H_6O \longrightarrow 2C + H_2O + 4H^+ + 4e^-$	+4	2	-2	0	+2
$C_6H_5O_7^{-3} + 9H^+ + 6e^- \longrightarrow 6C + 7H_2O$	-6	6	+1	0	-1
$C_{12}H_{22}O_{11} \longrightarrow 12C + 11H_2O$	0	12	0	0	0
$C_3H_8^{2+} \longrightarrow 3C + 8H^+ + 6e^-$	+6	3	-2	0	+2
$C_4H_8O^{2+} \longrightarrow 4C + 6H^+ + H_2O + 4e^-$	+4	4	-1	0	+1
$C_{10}H_{19}O_4^{3+} \longrightarrow 10C + 11H^+ + 4H_2O + 8e^-$	+8	10	$-\frac{4}{5}$	0	$+\frac{4}{5}$

The quantitative relationships among the substance-based concept of ONc, and the half reaction-based concepts of Te$^-$ and ΔONc are shown in Table 4.

Table 4. Relationships among ONc, Te^-, and ΔONc in a balanced half reaction

Redox term	Substance-based concept	Half reaction-based concept	
	ONc	ΔONc	Te^-
Half reaction	ONc (reactant) ⟶ ONc (product)	ΔONc = ONc (product) – ONc (reactant)	Te^- = nc × ΔONc
oxidation	increase	> 0 or (+)	> 0 or (+)
reduction	decrease	< 0 or (-)	< 0 or (-)
non-redox	no change	= 0	= 0

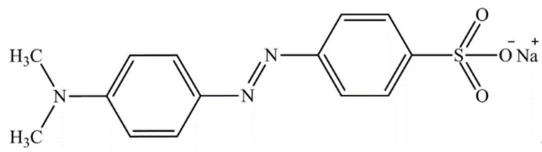
Based on the parameters in Table 4, by using the conversion of "$C_2H_4O + 2H^+ + 2e^- \longrightarrow C_2H_6O$" as an example, any one of the followings represents a half reduction reaction: (1) the criterium of Te^- = -2 (Te^- < 0; the gain of 2 electrons), (2) a decrease from ONc of C_2H_4O (reactant) = -1 to ONc of C_2H_6O (product) = -2, and (3) ΔONc = -1 (ΔONc < 0).

For another conversion of "$C_{10}H_{19}O_4^{3+} \longrightarrow 10C + 11H^+ + 4H_2O + 8e^-$", any one of the followings represents a half oxidation reaction: (1) Te^- = +8 (Te^- > 0; the loss of 8 electrons), (2) an increase from ONc of $C_{10}H_{19}O_4^{3+}$ (reactant) = $-\frac{4}{5}$ to ONc of C (product) = 0, and (3) ΔONc = $+\frac{4}{5}$ (ΔONc > 0).

8. C-atom Method: Alternative Procedures for $C_xH_yO_zX_wN_vS_uP_t$

There are three steps in the C-atom alternative procedures: fragmentation, balancing, and calculation. They are shown in the following examples.

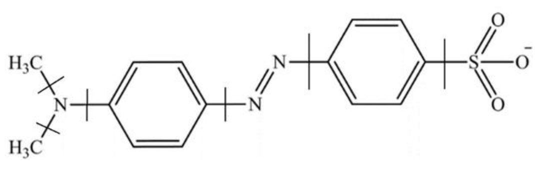
Example 11. Given the structural formula of methyl orange, $C_{14}H_{14}O_3N_3SNa$



$\longrightarrow C_{14}H_{14}O_3N_3S^- + Na^+$

(i) Fragmentation:

- break all C-heteroatom bonds: 3 C-N, 2 C-N, and 1 C-S
- eliminate all inorganic fragments: N^{-3}, $^-NN^-$, and $^-SO_3^-$
- identify the summation of all organic fragments

methyl orange		$C_{14}H_{14}O_3N_3S^-$
Inorganic fragments	N^{-3}, N_2^{-2}, SO_3^{-2}	$O_3N_3S^{-7}$
Summarized organic fragment	$(C_{14}H_{14}O_3N_3S^-) - (O_3N_3S^{-7})$	$C_{14}H_{14}^{+6}$

(ii) Balancing:

$C_{14}H_{14}^{+6} \longrightarrow C$

$C_{14}H_{14}^{+6} \longrightarrow 14C + 14H^+$

$C_{14}H_{14}^{+6} \longrightarrow 14C + 14H^+ + 8e^-$

Te^- = +8; nc = 14

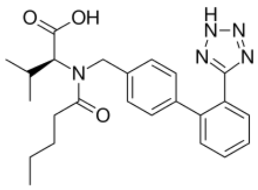
(iii) Calculation:

$$\text{ONc } (C_{14}H_{14}^{+6} \text{ or methyl orange}) = -\ \frac{Te^{-}}{nc}$$

$$= -\ \frac{(+8)}{14}$$

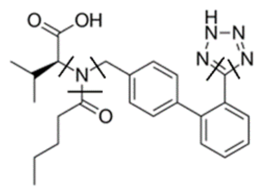
$$= -\ \frac{4}{7}$$

Example 12. Given the structural formula of Valsartan, $C_{24}H_{29}O_3N_5$



(i) Fragmentation:

- break all C-heteroatom bonds: 3 C-N, 1 C=N, and 1 C-N
- eliminate all inorganic fragments: N^{-3} and $^{-2}NNHNN^{-}$
- identify the summation of all organic fragments

Valsartan		$C_{24}H_{29}O_3N_5$
Inorganic fragments	N^{-3}, $NNHNN^{-3}$	HN_5^{-6}
Summarized organic fragment	$(C_{24}H_{29}O_3N_5) - (HN_5^{-6})$	$C_{24}H_{28}O_3^{+6}$

(ii) Balancing:

$C_{24}H_{28}O_3^{+6} \longrightarrow C$

$C_{24}H_{28}O_3^{+6} \longrightarrow 24C + 28H^{+} + 3O$

$C_{24}H_{28}O_3^{+6} + 6H^{+} \longrightarrow 24C + 28H^{+} + 3O + 6H^{+}$

$C_{24}H_{28}O_3^{+6} \longrightarrow 24C + 22H^{+} + 3H_2O$

$C_{24}H_{28}O_3^{+6} \longrightarrow 24C + 22H^{+} + 3H_2O + 16e^{-}$

$Te^{-} = +16$; $nc = 24$

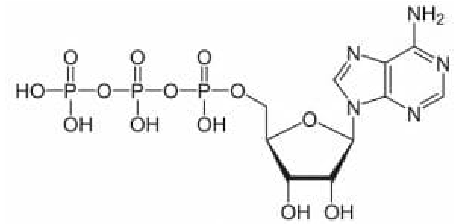
(iii) Calculation:

$$\text{ONc } (C_{24}H_{28}O_3^{+6} \text{ or Valsartan}) = -\ \frac{Te^{-}}{nc}$$

$$= -\ \frac{(+16)}{24}$$

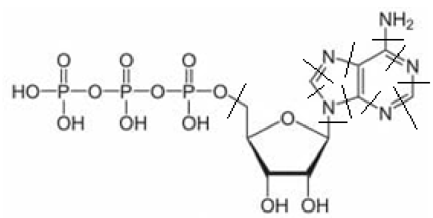
$$= -\ \frac{2}{3}$$

Example 13. Given the structural formula of ATP, $C_{10}H_{16}O_{13}N_5P_3$



(i) Fragmentation:

- break all C-heteroatom bonds: 1 C-O, 3 C-N, 1 C=N, 1 C-N, 1 C-N, 1 C=N, 1 C-N, 1C=N, and 1 C-N
- eliminate all inorganic fragments: $H_4P_3O_{10}^-$, $2N^{-3}$, NH_2^-, and $2N^{-3}$
- identify the summation of all organic fragments

ATP		$C_{10}H_{16}O_{13}N_5P_3$
Inorganic fragments	$H_4P_3O_{10}^-$, $2N^{-3}$, NH_2^-, $2N^{-3}$	$H_6O_{10}N_5P_3^{-14}$
Summarized organic fragment	$(C_{10}H_{16}O_{13}N_5P_3) – (H_6O_{10}N_5P_3^{-14})$	$C_{10}H_{10}O_3^{+14}$

(ii) Balancing:

$C_{10}H_{10}O_3^{+14} \longrightarrow C$

$C_{10}H_{10}O_3^{+14} \longrightarrow 10C + 10H^+ + 3O$

$C_{10}H_{10}O_3^{+14} + 6H^+ \longrightarrow 10C + 10H^+ + 3O + 6H^+$

$C_{10}H_{10}O_3^{+14} \longrightarrow 10C + 4H^+ + 3H_2O$

$C_{10}H_{10}O_3^{+14} + 10e^- \longrightarrow 10C + 4H^+ + 3H_2O$

$Te^- = -10$; nc = 10

(iii) Calculation:

$$ONc\ (C_{10}H_{10}O_3^{+14}\ \text{or ATP}) = -\ \frac{Te^-}{nc}$$

$$= -\ \frac{(-10)}{10}$$

$$= +1$$

9. Mathematical Equation to Count ONc for Organic Fragmentated $C_xH_yO_z^{charge}$

In examples 11 to 13, the organic fragments summarized above are presented in the general form of $C_xH_yO_z^{charge}$ (ON_H = +1 and ON_O = -2). Through the deduction from an organic fragmentated $C_xH_yO_z^{charge}$ to C, the general mathematical equation of ONc can be established.

$$C_xH_yO_z^{charge} \longrightarrow C$$

$$C_xH_yO_z^{charge} \longrightarrow xC + yH^+ + zO$$

$$C_xH_yO_z^{charge} + 2zH^+ \longrightarrow xC + yH^+ + zO + 2zH^+$$

$$C_xH_yO_z^{charge} \longrightarrow xC + (y\text{-}2z)H^+ + zH_2O$$

$$C_xH_yO_z^{charge} \longrightarrow xC + (y\text{-}2z)H^+ + zH_2O + (y\text{-}2z\text{-}charge)e^-$$

$$Te^- = (y\text{-}2z\text{-}charge);\ nc = x$$

$$ONc = -\frac{Te^-}{nc}$$

$$= -\frac{(y\text{-}2z\text{-}charge)}{x}$$

$$= \frac{charge-y+2z}{x}$$

The mathematical relationship between an organic fragmentated $C_xH_yO_z^{charge}$ and ONc is shown as $ONc = \frac{charge-y+2z}{x}$.

The ONc of $C_xH_yO_zX_wN_vS_uP_t$ in Examples 10 to 13 are recalculated and summarized in Table 5.

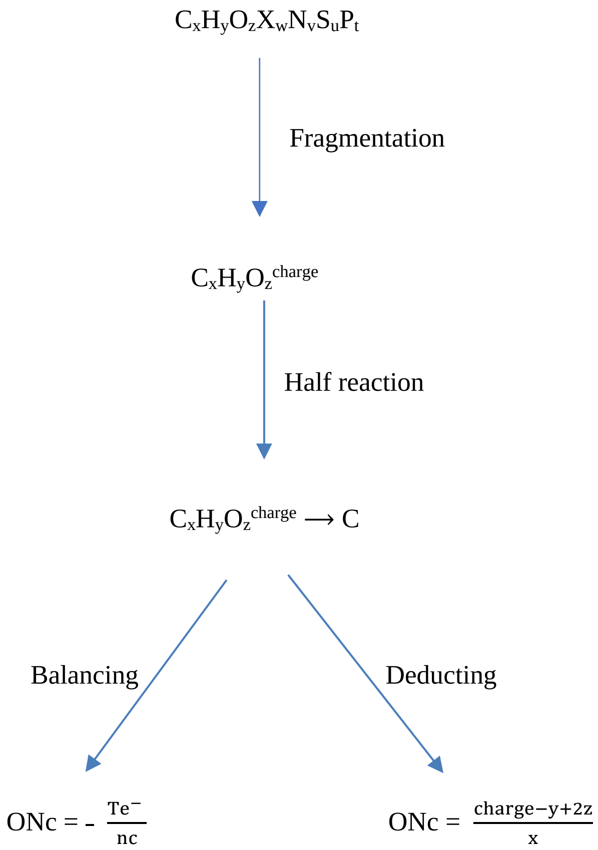
Table 5. Deducted mathematical equation for calculating ONc of organic fragmentated $C_xH_yO_z^{charge}$

$C_xH_yO_zX_wN_vS_uP_t$	$C_xH_yO_z^{charge}$	x	y	z	charge	$ONc = \frac{charge-y+2z}{x}$
Malathion, $C_{10}H_{19}O_6S_2P$	$C_{10}H_{19}O_4^{+3}$	10	19	4	+3	$ONc = \frac{(+3)\text{-}(19)+2(4)}{(10)} = -\frac{4}{5}$
methyl orange, $C_{14}H_{14}O_3N_3S^-$	$C_{14}H_{14}^{+6}$	14	14	0	+6	$ONc = \frac{(+6)\text{-}(14)+2(0)}{(14)} = -\frac{4}{7}$
Valsartan, $C_{24}H_{29}O_3N_5$	$C_{24}H_{28}O_3^{+6}$	24	28	3	+6	$ONc = \frac{(+6)\text{-}(28)+2(3)}{(24)} = -\frac{2}{3}$
ATP, $C_{10}H_{16}O_{13}N_5P_3$	$C_{10}H_{10}O_3^{+14}$	10	10	3	+14	$ONc = \frac{(+14)\text{-}(10)+2(3)}{(10)} = +1$

10. C-atom Method, Fragmentation Operation, and Organic Fragmentated $C_xH_yO_z^{charge}$

There are two developed pathways for the C-atom method, which are shown in Figure 1. Based on the C-atom method and the fragmentation operation, two new mathematical equations have been derived from an organic fragmentated $C_xH_yO_z^{charge}$. The first mathematical equation, $ONc = -\frac{Te^-}{nc}$, is derived by the balancing pathway. And the second one, $ONc = \frac{charge-y+2z}{x}$, is derived by the deducting pathway.

Figure 1. Scheme of the C-atom method: procedures and pathways



11. Conclusion

When there is no known structural information, the molecular formula method may not be able to assign mean oxidation number of organic carbons (ONc) to organic molecules or molecular ions. This article explores the carbon-atom method to overcome this problem. This method is developed as a reversed ion-electron method, which can balance a half reaction, count Te^- and nc, calculate ΔONc, and then assign ONc. The relationships among Te^-, ΔONc, and ONc can also be established. In addition, Te^-, ΔONc, or ONc can be used as a criterium for quantifying and understanding organic and bioorganic conversions. Two mathematical equations, $ONc = -\frac{Te^-}{nc}$ and $ONc = \frac{charge-y+2z}{x}$, are derived from counting ONc of an organic fragmentated $C_xH_yO_z^{charge}$. The mean ONc of any given organic or bioorganic compounds with known structural formulas can be effectively determined by using the carbon-atom method and the fragmentation operation.

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