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Simple mathematical equations for calculating oxidation number of organic carbons, number of transferred electrons, oxidative ratio, and mole of oxygen molecule in combustion reactions

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Research Article

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Simple mathematical equations for calculating oxidation number of organic carbons, number of transferred electrons, oxidative ratio, and mole of oxygen molecule in combustion reactions

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Abstract: The oxidation number and number of transferred electrons are two paramount parameters in the study of redox reactions. Their calculations are both important and challenging. The oxidation number of organic carbons is used in organic chemistry, biochemistry, and applied chemistry. Combustion reaction is a classical type of redox reaction, in which the oxygen molecule (O_2) is the oxidizing agent. In this article, the integration of three sets of relations is explored by using the method of balancing organic combustion: (i) number of transferred electrons and oxidation number of organic carbons, (ii) mole of oxygen molecule and number of transferred electrons, and (iii) oxidative ratio, oxidation number of organic carbons, and number of transferred electrons. This method can also establish the relationships among the stoichiometric coefficients, mole of oxygen molecule, oxidative ratio, number of transferred electrons, and oxidation number of organic carbons. Furthermore, the oxidation number of organic carbons and the number of transferred electrons of a given organic compound can be determined by the derived mathematical equations.

Keywords: organic carbons; organic combustion reaction; oxidation number; oxidative ratio; oxygen molecule (O_2); transferred electrons.

Introduction

The balancing of chemical equations, stoichiometry, and redox reactions are some of the basic contents in chemistry curriculum (Chang & Goldsby, 2013; Tro, 2020). Redox reaction is an electron-transfer reaction, and it emerges with the oxidation number change (ΔON). The oxidation number (ON) and the number of transferred electrons (Te^-) are two paramount parameters in the study of redox reactions (IUPAC, 2019). The oxidation number of organic carbons (ON_C) is widely used in the fields of organic and biological chemistry (Bentley, Franzen, & Chasteen, 2002; Hanson, 1990; Halkides, 2000; Yuen & Lau, 2022a), environmental chemistry (Kroll et al., 2011; Kroll, Lim, Kessler, & Wilson, 2015), and biogeochemistry (Chadwick, Masiello, Baldock, Smernik, & Randerson, 2007; Chadwick, Masiello, Baldock, Smernik, & Randerson, 2007; Dick, Yu, Tan, & Lu, 2019; Masiello, Hockaday, & Gallagher, 2007).

The net primary production (NPP) reactions and combustion reactions are two opposite redox reactions. Examples are shown as follows:

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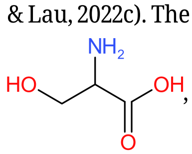
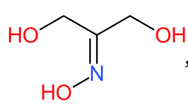
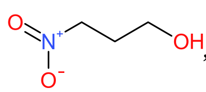
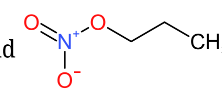
Net primary production reaction: $CO_2 + H_2O$ + N-resource $\rightarrow C_xH_yO_zN_v + O_2$
Combustion reaction: $C_xH_yO_zN_v + O_2 \rightarrow CO_2 + H_2O$ + N-product

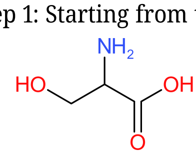
The oxidative ratio (OR) is defined as the ratio of moles of O_2 to moles of CO_2 in NPP and combustion reactions (Gallagher et al., 2014; Randerson et al., 2006; Worrall, Clay, Masiello, & Mynheer, 2013). The relationship between OR and ON_C has been established in the study of NPP reactions (Hockaday et al., 2009, 2015; Masiello, Gallagher, Randerson, Deco, & Chadwick, 2008), and the relationships among OR, ON_C, and Te^- have been found in the study of organic combustion reactions (Yuen & Lau, 2022b). Although the stoichiometric amount of oxygen molecule (nO_2) plays a significant role in NPP and combustion reactions, the relationships among nO_2, OR, Te^-, and ON_C have not been revealed.

Assigning ON and counting Te^- are important tasks in the study of redox reactions and they often pose difficulties for teachers and students (Brandriet & Bretz, 2014; De Jong, Acampo, & Verdonk, 1995; Garnett & Treagust, 1992). The purpose of this article is to explore a method which can solve the aforesaid problems. A combustion model is established to understand the relationships among ON_C, Te^-, nO_2, and OR. Three pillars are needed. First, an organic combustion reaction acts as a model reaction. Second, the method of balancing and deducting chemical equations is used as a tool. Third, the stoichiometric coefficients (SC) in the balanced combustion reaction are used as connectors. Three sets of relations: (i) OR, ON_C, and Te^-; (ii) ON_C and Te^-; and (iii) nO_2 and Te^- are integrated. Consequently, new interrelationships among nO_2, OR, Te^-, and ON_C are established. The Te^- and ON_C of organic compounds can also be determined by the derived mathematical equations.

Procedures for counting OR, Te^-, and ON_C of organic molecules

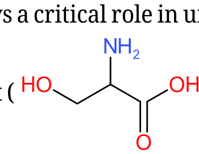
The ON_C of organonitrogen are seldom studied (Kauffman, 1986; Jurowski, Krzeczkowska, & Jurowska, 2015; Yuen & Lau, 2022c). The general formula of organonitrogen compound, $C_xH_yO_zN_v$, is chosen as an example. Even though , , , and  have the same molecular formula of $C_3H_7O_3N$, these four structural formulas have different ON_N.

Example 1. Balancing the combustion reaction of $C_3H_7O_3N$.
Step 1: Starting from the structural formula of $C_3H_7O_3N$.



Counting ON for non-carbon atoms:
All hydrogen atoms: $ON_H = +1$.
All oxygen atoms: $ON_O = -2$.
One nitrogen atom: $ON_N = -3$.

Step 2: Setting up the combustion reaction.

The N-product plays a critical role in understanding the stoichiometric relationship in a combustion reaction. The ON_N of the reactant () is identified as −3, and the NH_3 ($ON_N = -3$) is selected as the N-product accordingly.

The combustion reaction is shown as: $C_3H_7O_3N \rightarrow CO_2 + H_2O + NH_3$.

Step 3: Balancing the combustion reaction.

The combustion reaction is balanced by balancing atoms in the sequence from C atoms to N atoms to H atoms to O atoms.

$$\text{balancing C: } C_3H_7O_3N + O_2 \rightarrow 3CO_2 + H_2O + NH_3$$

$$\text{balancing N: } C_3H_7O_3N + O_2 \rightarrow 3CO_2 + H_2O + NH_3$$

$$\text{balancing H: } C_3H_7O_3N + O_2 \rightarrow 3CO_2 + 2H_2O + NH_3$$

$$\text{balancing O: } C_3H_7O_3N + \frac{5}{2}O_2 \rightarrow 3CO_2 + 2H_2O + NH_3$$

Step 4: Identifying the stoichiometric coefficients of nO_2 and nCO_2.

Based on the balanced combustion reaction, the coefficients of $nO_2 = \frac{5}{2}$ and $nCO_2 = 3$ can be identified.

Step 5: Counting OR from the ratio of nO_2 to nCO_2.

Based on the ratio of nO_2 to nCO_2 $\left(\frac{nO_2}{nCO_2}\right)$, the OR = $\frac{5}{6}$ can be determined.

Step 6: Counting Te^- from nO_2.

O_2 is the oxidizing agent in the combustion reactions. Each O atom gains 2 electrons ($O + 2e^- \rightarrow O^{-2}$) and each O_2 molecule gains 4 electrons ($O_2 + 4e^- \rightarrow 2O^{-2}$).

$$Te^- = 4\,nO_2$$

$$Te^- = 4\left(\frac{5}{2}\right) = 10 \text{ (electrons)}$$

Step 7: Counting ON_C from Te^-.

The relationship between Te^- and ΔON_C has been established in the half redox reactions (Yuen & Lau, 2022d). The mathematical equations and calculation are shown as follows:

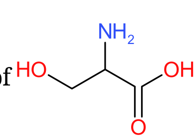
$$Te^- = n_C\,\Delta ON_C$$

$$\Delta ON_C = \frac{Te^-}{n_c}$$

$$\Delta ON_C = ON_C\,(CO_2) - ON_C\,(C_3H_7O_3N)$$

$$\Delta ON_C = 4 - ON_C\,(C_3H_7O_3N)$$

$$\begin{aligned} ON_C\,(C_3H_7O_3N) &= 4 - \frac{Te^-}{n_c} \\ &= 4 - \frac{10}{3} \\ &= +\frac{2}{3} \end{aligned}$$

The mean ON_C of 

($C_3H_7O_3N$) equals to $+\frac{2}{3}$.

Balancing combustion reactions: counting nO_2, nCO_2, OR, Te^-, and ON_C

Nitrogen atoms have nine oxidation numbers (ON_N), the values of which lie between −3 to +5. By using the same procedure as shown in Example 1 (ON_N = −3), different N-products are assigned by different ON_N. The chemical

Table 1: Parameters of ON_N, nO_2, nCO_2, OR, Te^-, and ON_C in the balancing combustion reactions of $C_3H_7O_3N$ molecules.

Equation #	Balancing the combustion reaction	ON_N	nO_2	nCO_2	OR	Te^-	ONc
1	$C_3H_7O_3N + \frac{5}{2}O_2 \rightarrow 3CO_2 + 2H_2O + NH_3$	−3	$\frac{5}{2}$	3	$\frac{5}{6}$	10	$+\frac{2}{3}$
2	$C_3H_7O_3N + \frac{11}{4}O_2 \rightarrow 3CO_2 + \frac{5}{2}H_2O + \frac{1}{2}N_2H_4$	−2	$\frac{11}{4}$	3	$\frac{11}{12}$	11	$+\frac{1}{3}$
3a	$C_3H_7O_3N + 3O_2 \rightarrow 3CO_2 + 3H_2O + \frac{1}{2}N_2H_2$	−1	3	3	1	12	0
3b	$C_3H_7O_3N + 3O_2 \rightarrow 3CO_2 + 2H_2O + NH_2OH$	−1	3	3	1	12	0
4	$C_3H_7O_3N + \frac{13}{4}O_2 \rightarrow 3CO_2 + \frac{7}{2}H_2O + \frac{1}{2}N_2$	0	$\frac{13}{4}$	3	$\frac{13}{12}$	13	$-\frac{1}{3}$
5	$C_3H_7O_3N + \frac{7}{2}O_2 \rightarrow 3CO_2 + \frac{7}{2}H_2O + \frac{1}{2}N_2O$	+1	$\frac{7}{2}$	3	$\frac{7}{6}$	14	$-\frac{2}{3}$
6	$C_3H_7O_3N + \frac{15}{4}O_2 \rightarrow 3CO_2 + \frac{7}{2}H_2O + NO$	+2	$\frac{15}{4}$	3	$\frac{5}{4}$	15	1
7a	$C_3H_7O_3N + 4O_2 \rightarrow 3CO_2 + 3H_2O + HNO_2$	+3	4	3	$\frac{4}{3}$	16	$-\frac{4}{3}$
7b	$C_3H_7O_3N + 4O_2 \rightarrow 3CO_2 + \frac{7}{2}H_2O + \frac{1}{2}N_2O_3$	+3	4	3	$\frac{4}{3}$	16	$-\frac{4}{3}$
8	$C_3H_7O_3N + \frac{17}{4}O_2 \rightarrow 3CO_2 + \frac{7}{2}H_2O + \frac{1}{2}NO_2$	+4	$\frac{17}{4}$	3	$\frac{17}{12}$	17	$-\frac{5}{3}$
9a	$C_3H_7O_3N + \frac{9}{2}O_2 + 3CO_2 + 3H_2O + HNO_3$	+5	$\frac{9}{2}$	3	$\frac{3}{2}$	18	−2
9b	$C_3H_7O_3N + \frac{9}{2}O_2 \rightarrow 3CO_2 + \frac{7}{2}H_2O + \frac{1}{2}N_2O_5$	+5	$\frac{9}{2}$	3	$\frac{3}{2}$	18	−2

formulas of N-products are combined with H-atom, O-atom, or both O-atom and H-atom. The resulted values of nO_2, nCO_2, OR, Te^-, and ON_C are given in Table 1.

When Equations (1) and (2) are compared, NH_3 and N_2H_4 are found to have different ON_N, and they produce different nO_2, OR, and Te^-.

$$C_3H_7O_3N + \frac{5}{2}\,O_2 \rightarrow 3CO_2 + 2H_2O + NH_3 \tag{1}$$

$$C_3H_7O_3N + \frac{11}{4}\,O_2 \rightarrow 3CO_2 + \frac{5}{2}\,H_2O + \frac{1}{2}\,N_2H_4 \tag{2}$$

When Equations (3) and (4) are compared, N-products of HNO_3 and N_2O_5 are found to contain the same ON_N even though they have different chemical formulas. Their nO_2, OR, and Te^- remain the same.

$$C_3H_7O_3N + \frac{9}{2}\,O_2 \rightarrow 3CO_2 + 3H_2O + HNO_3 \tag{3}$$

$$C_3H_7O_3N + \frac{9}{2}\,O_2 \rightarrow 3CO_2 + \frac{7}{2}\,H_2O + \frac{1}{2}\,N_2O_5 \tag{4}$$

Balancing general combustion reactions: counting nO_2, nCO_2, OR, Te^-, and ON_C by using SC

$$C_xH_yO_zN_v + O_2 \rightarrow CO_2 + H_2O + N\text{ - product}$$

$C_xH_yO_zN_v$ is used for balancing and deducting the combustion equation. NH_3 (ON_N = −3) is chosen as a N-product in Example 2.

Example 2. Balancing the general combustion reaction of $C_xH_yO_zN_v$.

(a) Balancing the combustion reaction: $C_xH_yO_zN_v + O_2 \rightarrow CO_2 + H_2O + NH_3$.

$$\text{balancing C: } C_xH_yO_zN_v + O_2 \rightarrow xCO_2 + H_2O + NH_3$$

$$\text{balancing N: } C_xH_yO_zN_v + O_2 \rightarrow xCO_2 + H_2O + \mathrm{v}NH_3$$

$$\text{balancing H: } C_xH_yO_zN_v + O_2 \rightarrow xCO_2 + \frac{y-3v}{2}\,H_2O + vNH_3$$

$$\text{balancing O : } C_xH_yO_zN_v + \frac{4x+y-2z-3v}{4}\,O_2 \rightarrow xCO_2 + \frac{y-3v}{2}\,H_2O + vNH_3$$

(b) Expressing nO_2, nCO_2, OR, Te^-, and ON_C by using SC.

$$nO_2 = \frac{4x+y-2z-3v}{4}$$

$$nCO_2 = n_C = x$$

$$OR = \frac{nO_2}{nCO_2} = \frac{4x+y-2z-3v}{4x}$$

$$Te^- = 4\,nO_2 = 4x+y-2z-3v$$

$$ON_C = 4 - \frac{Te^-}{x} = 4 - \frac{4x+y-2z-3v}{x} = \frac{-y+2z+3v}{x}$$

By using the same procedure shown in Example 2, different N-products are assigned by different ON_N. Their values of ON_N, nO_2, OR, Te^-, and ON_C are given in Table 2.

Table 2: Stoichiometric coefficients and parameters of ON_N, nO_2, OR, Te^-, and ON_C in the balancing combustion reactions of $C_xH_yO_zN_v$ molecules.

Balancing the combustion reaction	ON_N	nO_2	OR	Te^-	ON_C
$C_xH_yO_zN_v + \frac{4x+y-2z-3v}{4}O_2 \rightarrow xCO_2 + vNH_3 + \frac{y-3v}{2}H_2O$	−3	$\frac{4x+y-2z-3v}{4}$	$\frac{4x+y-2z-3v}{4x}$	$4x+y-2z-3v$	$\frac{-y+2z+3v}{x}$
$C_xH_yO_zN_v + \frac{4x+y-2z-2v}{4}O_2 \rightarrow xCO_2 + \frac{v}{2}N_2H_4 + \frac{y-2v}{2}H_2O$	−2	$\frac{4x+y-2z-2v}{4}$	$\frac{4x+y-2z-2v}{4x}$	$4x+y-2z-2v$	$\frac{-y+2z+2v}{x}$
$C_xH_yO_zN_v + \frac{4x+y-2z-v}{4}O_2 \rightarrow xCO_2 + \frac{v}{2}N_2H_2 + \frac{y-v}{2}H_2O$	−1	$\frac{4x+y-2z-v}{4}$	$\frac{4x+y-2z-v}{4x}$	$4x+y-2z-v$	$\frac{-y+2z+v}{x}$
$C_xH_yO_zN_v + \frac{4x+y-2z-v}{4}O_2 \rightarrow xCO_2 + vNH_2OH + \frac{y-3v}{2}H_2O$	−1	$\frac{4x+y-2z-v}{4}$	$\frac{4x+y-2z-v}{4x}$	$4x+y-2z-v$	$\frac{-y+2z+v}{x}$
$C_xH_yO_zN_v + \frac{4x+y-2z}{4}O_2 \rightarrow xCO_2 + \frac{v}{2}N_2 + \frac{y}{2}H_2O$	0	$\frac{4x+y-2z}{4}$	$\frac{4x+y-2z-3v}{4x}$	$4x+y-2z$	$\frac{-y+2z}{x}$
$C_xH_yO_zN_v + \frac{4x+y-2z+v}{4}O_2 \rightarrow xCO_2 + \frac{v}{2}N_2O + \frac{y}{2}H_2O$	+1	$\frac{4x+y-2z+v}{4}$	$\frac{4x+y-2z+v}{4x}$	$4x+y-2z+v$	$\frac{-y+2z-v}{x}$
$C_xH_yO_zN_v + \frac{4x+y-2z+2v}{4}O_2 \rightarrow xCO_2 + vNO + \frac{y}{2}H_2O$	+2	$\frac{4x+y-2z+2v}{4}$	$\frac{4x+y-2z+2v}{4x}$	$4x+y-2z+2v$	$\frac{-y+2z-2v}{x}$
$C_xH_yO_zN_v + \frac{4x+y-2z+3v}{4}O_2 \rightarrow xCO_2 + vHNO_2 + \frac{y-v}{2}H_2O$	+3	$\frac{4x+y-2z+3v}{4}$	$\frac{4x+y-2z+3v}{4x}$	$4x+y-2z+3v$	$\frac{-y+2z-3v}{x}$
$C_xH_yO_zN_v + \frac{4x+y-2z+3v}{4}O_2 \rightarrow xCO_2 + \frac{v}{2}N_2O_3 + \frac{y}{2}H_2O$	+3	$\frac{4x+y-2z+3v}{4}$	$\frac{4x+y-2z+3v}{4x}$	$4x+y-2z+3v$	$\frac{-y+2z-3v}{x}$
$C_xH_yO_zN_v + \frac{4x+y-2z+4v}{4}O_2 \rightarrow xCO_2 + vNO_2 + \frac{y}{2}H_2O$	+4	$\frac{4x+y-2z+4v}{4}$	$\frac{4x+y-2z+4v}{4x}$	$4x+y-2z+4v$	$\frac{-y+2z-4v}{x}$
$C_xH_yO_zN_v + \frac{4x+y-2z+5v}{4}O_2 \rightarrow xCO_2 + vHNO_3 + \frac{y-v}{2}H_2O$	+5	$\frac{4x+y-2z+5v}{4}$	$\frac{4x+y-2z+5v}{4x}$	$4x+y-2z+5v$	$\frac{-y+2z-5v}{x}$
$C_xH_yO_zN_v + \frac{4x+y-2z+5v}{4}O_2 \rightarrow xCO_2 + \frac{v}{2}N_2O_5 + \frac{y}{2}H_2O$	+5	$\frac{4x+y-2z+5v}{4}$	$\frac{4x+y-2z+5v}{4x}$	$4x+y-2z+5v$	$\frac{-y+2z-5v}{x}$

Formulating nO_2, nCO_2, OR, Te^-, and ON_C of $C_xH_yO_zN_v$ molecule

Any non-carbon ON (ON_H, ON_O, ON_N) of $C_xH_yO_zN_v$ can be determined by its structural formula (Yuen & Lau, 2022c). Its atomic coefficients can also be identified.

non-carbon ON: ON_H, ON_O, ON_N.

atomic coefficient: x for carbon, y for hydrogen, z for oxygen, v for nitrogen.

Atom	C	H	O	N
ON	–	ON_H	ON_O	ON_N
Atomic coefficient	x	y	z	v

By balancing the combustion reaction of $C_xH_yO_zN_v + O_2 \rightarrow CO_2 + H_2O$ + [N-product], the general mathematical equations of $C_xH_yO_zN_v$ molecules are given as follows:

$$nO_2 = \frac{Te^-}{4} = \frac{4x + ON_H(y) + ON_O(z) + ON_N(v)}{4}$$

$$Te^- = 4\,nO_2 = 4x + ON_H(y) + ON_O(z) + ON_N(v)$$

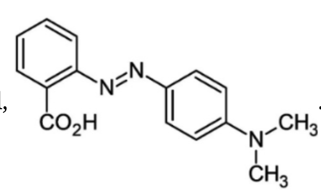
$$nCO_2 = n_C = x$$

$$OR = \frac{nO_2}{nCO_2} = \frac{Te^-}{4x} = \frac{4x + ON_H(y) + ON_O(z) + ON_N(v)}{4x}$$

$$ON_C = 4 - \frac{Te^-}{x} = \frac{-ON_H(y) - ON_O(z) - ON_N(v)}{x}$$

The values of nO_2, Te^-, nCO_2, OR, and ON_C can be calculated by using non-carbon ON of ON_H, ON_O, and ON_N, and atomic coefficients of x, y, z, and v.

Procedures for determining Te^-, nO_2, nCO_2, OR, and ON_C of $C_xH_yO_zN_v$ molecule and balancing its corresponding combustion reaction

Example 3. Given methyl red, .

(a) Determining all non-carbon ON and atomic coefficients from the structural formula.

$$C_x\,H_y\,O_z\,N_v = C_{15}\,H_{15}\,O_2\,N_3$$

$$ON_H = +1, ON_O = -2, ON_N = -1, ON_N = -3$$

$$x = 15,\ y = 15,\ z = 2, v_1 = 2, v_2 = 1$$

Atom	C	H	O	N	N
ON	–	+1	−2	−1	−3
Atomic coefficient	15	15	2	2	1

(b) Calculating Te^-, nO_2, nCO_2, OR, and ON_C by using mathematical equations.

Mathematical equation	Calculation
$Te^- = 4x + ON_H(y) + ON_O(z) + ON_N(v_1) + ON_N(v_2)$	$Te^- = 4(15) + (+1)(15) + (-2)(2) + (-1)(2) + (-3)(1) = 66$
$nO_2 = \frac{Te^-}{4}$	$nO_2 = \frac{Te^-}{4} = \frac{66}{4} = \frac{33}{2}$
$nCO_2 = n_C = x$	$nCO_2 = 15$
$OR = \frac{Te^-}{4x}$	$OR = \frac{Te^-}{4x} = \frac{66}{4(15)} = \frac{11}{10}$
$ON_C = 4 - \frac{Te^-}{x}$	$ONc = 4 - \frac{Te^-}{x} = 4 - \frac{66}{15} = -\frac{6}{15}$

(c) Balancing the combustion reaction by using the SC of nO_2 and nCO_2.

The unbalanced combustion reaction of "$C_{15}H_{15}O_2N_3 + O_2 \rightarrow CO_2 + H_2O + N_2H_2 + NH_3$" can be set up and balanced as follows:

Using the calculated SC of nO_2 and nCO_2:

$$C_{15}H_{15}O_2N_3 + \frac{33}{2}O_2 \rightarrow 15CO_2 + H_2O + N_2H_2 + NH_3$$

Balancing N_2H_2 and NH_3:

$$C_{15}H_{15}O_2N_3 + \frac{33}{2}\,O_2 \rightarrow 15CO_2 + H_2O + N_2H_2 + NH_3$$

Balancing H_2O:

$$C_{15}H_{15}O_2N_3 + \frac{33}{2}O_2 \rightarrow 15CO_2 + 5H_2O + N_2H_2 + NH_3$$

In Example 3, the values of Te^-, nO_2, OR, and ON_C can be calculated by the derived mathematical equations, which are based on the balanced organic combustion reactions. Reversely, the combustion reaction of $C_xH_yO_zN_v$ molecules can also be balanced by the resulted nO_2 and nCO_2.

Interrelationships among Te^-, nO_2, OR, and ON_C in $C_xH_yO_zX_wN_vS_uP_t$ molecule

The strategy, which is used for balancing and deducting $C_xH_yO_zN_v$, can be extended to work on $C_xH_yO_zX_wN_vS_uP_t$ molecule (X, N, S, P stand for halogen, nitrogen, sulfur, and phosphorus respectively). For $C_xH_yO_zX_wN_vS_uP_t$, all possible non-carbon ON are shown as: $ON_H = +1$, $ON_O = -1$ to -2, $ON_X = -1$ to $+7$, $ON_N = -3$ to $+5$, $ON_S = -2$ to $+6$, and $ON_P = -3$ to $+5$.

The general combustion reaction: $C_xH_yO_zX_wN_vS_uP_t + O_2 \rightarrow CO_2 + H_2O + [\text{O - product}] + [\text{X - product}] + [\text{N - product}] + [\text{S - product}] + [\text{P - product}]$.

(a) ON and atomic coefficients for calculating Te^-, nO_2, nCO_2, OR, and ON_C.

non-carbon ON: ON_H, ON_O, ON_X, ON_N, ON_S, ON_P.

atomic coefficients: x, y, z, w, v, u, t.

Atom	C	H	O	X	N	S	P
ON		ON_H	ON_O	ON_X	ON_N	ON_S	ON_P
Atomic coefficient	x	y	z	w	v	u	t

The derived general mathematical equations for $C_xH_yO_zX_wN_vS_uP_t$ are shown as follows:

$$Te^- = 4x + ON_H(y) + ON_O(z) + ON_X(w) + ON_N(v) + ON_S(u) + ON_P(t)$$

$$nO_2 = \frac{Te^-}{4} = \frac{4x + ON_H(y) + ON_O(z) + ON_X(w) + ON_N(v) + ON_S(u) + ON_P(t)}{4}$$

$$nCO_2 = n_C = x$$

$$OR = \frac{Te^-}{4x} = \frac{4x + ON_H(y) + ON_O(z) + ON_X(w) + ON_N(v) + ON_S(u) + ON_P(t)}{4x}$$

$$ON_C = 4 - \frac{Te^-}{x} = \frac{-ON_H(y) - ON_O(z) - ON_X(w) - ON_N(v) - ON_S(u) - ON_P(t)}{x}$$

(b) Relationships among SC, nO_2, OR, Te^-, and ON_C.

By using combustion reactions as models, the relationships among nO_2, OR, Te^-, and ON_C are derived. The tetrahedral model with SC in the center as connectors can be established and is shown in Figure 1.

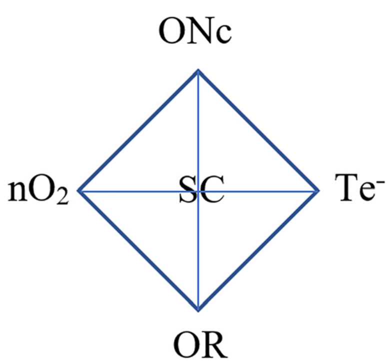


Figure 1: Tetrahedral relationships among nO_2, OR, Te^-, and ON_C with SC in the center.

By integrating three sets of relationships of (i) OR and Te^-; (ii) ON_C and Te^-; and (iii) nO_2 and Te^-, the interrelationships among four parameters of nO_2, OR, Te^-, and ON_C are established. As a result, there are six sets of relationships among four parameters: nO_2, OR, Te^-, and ON_C, which are derived and summarized in Table 3.

Table 3: Interrelationships among four parameters: nO_2, OR, Te^-, and ON_C.

Relationship	Mathematical equation	
Te^- and nO_2	$Te^- = 4\ nO_2$	$nO_2 = \frac{Te^-}{4}$
Te^- and OR	$Te^- = 4^{x}$ OR	$OR = \frac{Te^-}{4x}$
Te^- and ONc	$Te^- = x\,(4 - ON_C)$	$ON_C = 4 - \frac{Te^-}{x}$
ON_C and nO_2	$ON_C = 4\,(1 - \frac{nO_2}{x})$	$nO_2 = \frac{x}{4}(4 - ON_C)$
ON_C and OR	$ON_C = 4\,(1 - OR)$	$OR = 1 - \frac{ON_C}{4}$
nO_2 and OR	$nO_2 = x$ OR	$OR = \frac{nO_2}{x}$

$x = n_C$ = atomic coefficient of organi c carbons in $C_xH_yO_zX_wN_vS_uP_t$ molecule.

(c) Triangular relationships among Te^-, OR, and ON_C.

The Te^-, OR, or ON_C can be determined by nO_2. The triangular relationship among Te^-, OR, and ON_C with nO_2 in the center is shown in Figure 2.

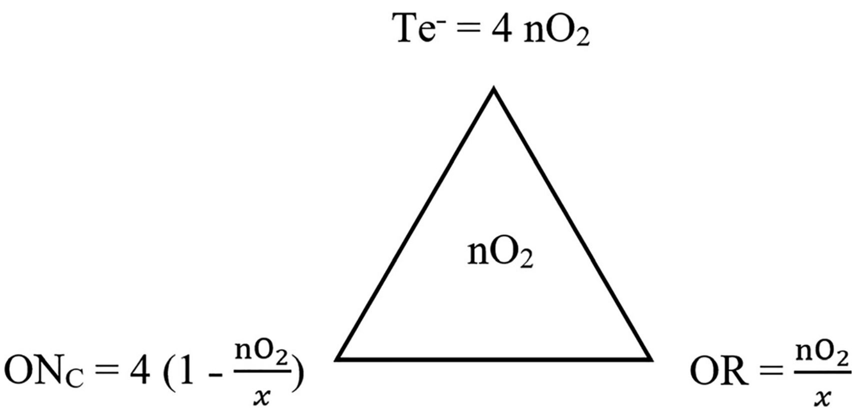


Figure 2: Triangular relationships among Te^{-}, OR, and ON_C with nO_2 in the center.

(d) Triangular relationships among nO_2, ON_C, and Te^{-}.

The nO_2, ON_C, and Te^{-} can be determined by OR. The triangular relationship among nO_2, ON_C, and Te^{-} with OR in the center is shown in Figure 3.

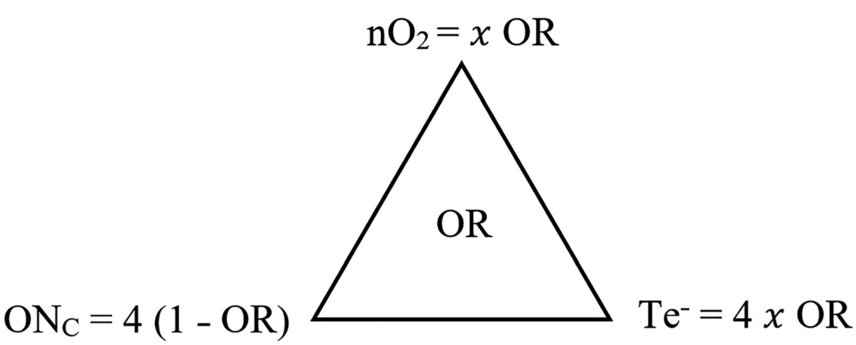
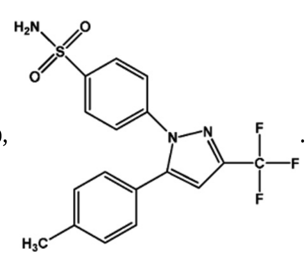


Figure 3: Triangular relationships among nO_2, ON_C, and Te^{-} with OR in the center.

(e) Equivalence between the gain of electrons and the loss of electrons.

By using the combustion model, the gain of electrons from oxygen molecules (O_2) and the loss of electrons from carbon atoms of $C_xH_yO_zX_wN_vS_uP_t$ molecule must be equal. It means that for all other atoms, their ON do not change in the combustion reaction.

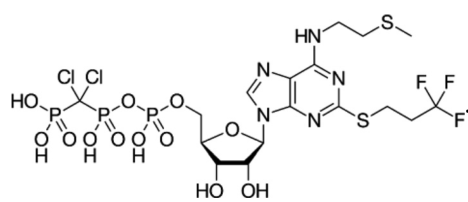
Determining Te^{-}, nO_2, OR, and ON_C of $C_xH_yO_zX_wN_vS_uP_t$ molecule by using mathematical equations

Example 4. Given Celecoxib,  .

$C_xH_yO_zX_wN_vS_u = C_{17}H_{14}O_2F_3N_3S$.
$ON_H = +1, ON_O = -2, ON_F = -1, ON_N = -3, ON_N = -2, ON_S = +4$
$x = 17, y = 14, z = 2, w = 3, v_1 = 1, v_2 = 2, u = 1$

Atom	C	H	O	F	N	N	S
ON	–	+1	−2	−1	−3	−2	+4
Atomic coefficient	17	14	2	3	1	2	1

Mathematical equation	**Calculation**
$Te^- = 4x + ON_H(y) + ON_O(z) + ON_X(w) + ON_N(v1) + ON_N(v2) + ON_S(u)$	$Te^- = 4(17) + (+1)(14) + (-2)(2) + (-1)(3) + (-3)(1) + (-2)2 + (+4)(1) = 72$
$nO_2 = \frac{Te^-}{4}$	$nO_2 = \frac{Te^-}{4} = \frac{72}{4} = 18$
$nCO_2 = n_C = x$	$nCO_2 = 17$
$OR = \frac{Te^-}{4x}$	$OR = \frac{Te^-}{4x} = \frac{72}{4(17)} = \frac{18}{17}$
$ON_C = 4 - \frac{Te^-}{x}$	$ON_C = 4 - \frac{Te^-}{x} = 4 - \frac{72}{17} = -\frac{4}{17}$

Example 5. Given Cangrelor, 

$C_xH_yO_zX_wN_vS_uP_t = C_{17}H_{25}O_{12}Cl_2F_3N_5S_2P_3$
$ON_H = +1, ON_O = -2, ON_F = -1, ON_{Cl} = -1, ON_N = -3, ON_S = -2, ON_P = +5$
$x = 17, y = 25, z = 12, w_1 = 2, w_2 = 3, v = 5, u = 2, t = 3$

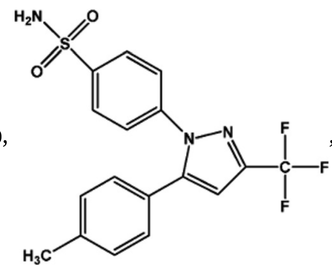
Atom	C	H	O	Cl	F	N	S	P
ON	–	+1	−2	−1	−1	−3	−2	+5
Atomic coefficient	17	25	12	2	3	5	2	3

Mathematical equation	**Calculation**
$Te^- = 4x + ON_H(y) + ON_O(z) + ON_{Cl}(w_1) + ON_F(w_2) + ON_N(v) + ON_S(u) + ON_P(t)$	$Te^- = 4(17) + (+1)(25) + (-2)(12) + (-1)(2) + (-1)(3) + (-3)(5) + (-2)2 + (+5)(3) = 60$
$nO_2 = \frac{Te^-}{4}$	$nO_2 = \frac{Te^-}{4} = \frac{60}{4} = 15$
$nCO_2 = n_C = x$	$nCO_2 = 17$
$OR = \frac{Te^-}{4x}$	$OR = \frac{Te^-}{4} = \frac{60}{4(17)} = \frac{15}{17}$
$ON_C = 4 - \frac{Te^-}{x}$	$ON_C = 4 - \frac{Te^-}{x} = 4 - \frac{60}{17} = +\frac{8}{17}$

In Examples 4 and 5, the mathematical equation for counting Te^- of organic compounds in the general chemical formula of $C_xH_yO_zX_wN_vS_uP_t$ is used and then nO_2, OR, and ON_C can be calculated consequently.

Procedures for balancing combustion reactions of $C_xH_yO_zX_wN_vS_uP_t$ molecule and determining its corresponding Te^- and ON_C from nO_2 or OR

Example 6. Given Celecoxib,



, $C_{17}H_{14}O_2F_3N_3S$.

(a) Determining all non-carbon ON and all atomic coefficients.

Atom	C	H	O	F	N	N	S
ON	–	+1	−2	−1	−2	−3	+4
Atomic coefficient	17	14	2	3	2	1	1

(b) Balancing the combustion reaction

The unbalanced combustion reaction of "$C_{17}H_{14}O_2F_3N_3S + O_2 \rightarrow CO_2 + H_2O + HF + H_2NNH_2 + NH_3 + SO_2$" can be set up and balanced as follows:

Using the coefficient of nCO_2 ($n_C = nCO_2$):

$$C_{17}H_{14}O_2F_3N_3S + O_2 \rightarrow 17CO_2 + H_2O + HF + H_2NNH_2 + NH_3 + SO_2$$

Balancing HF:

$$C_{17}H_{14}O_2F_3N_3S + O_2 \rightarrow 17CO_2 + H_2O + 3HF + H_2NNH_2 + NH_3 + SO_2$$

Balancing H_2NNH_2 and NH_3:

$$C_{17}H_{14}O_2F_3N_3S + O_2 \rightarrow 17CO_2 + H_2O + 3HF + H_2NNH_2 + NH_3 + SO_2$$

Balancing SO_2:

$$C_{17}H_{14}O_2F_3N_3S + O_2 \rightarrow 17CO_2 + H_2O + 3HF + H_2NNH_2 + NH_3 + SO_2$$

Balancing H_2O:

$$C_{17}H_{14}O_2F_3N_3S + O_2 \rightarrow 17CO_2 + 2H_2O + 3HF + H_2NNH_2 + NH_3 + SO_2$$

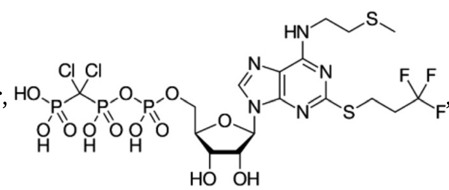
Balancing O_2:

$$C_{17}H_{14}O_2F_3N_3S + 18O_2 \rightarrow 17CO_2 + 2H_2O + 3HF + H_2NNH_2 + NH_3 + SO_2$$

$nO_2 = 18$	$nCO_2 = 17$	$OR = \frac{18}{17}$

(c) Calculating Te^- and ON_C from nO_2 or OR

Calculating Te^- and ONc			
From nO_2		**From OR**	
Mathematical equation	**Calculation**	**Mathematical equation**	**Calculation**
$Te^- = 4\ nO_2$	$Te^- = 4\ (18) = 72$	$Te^- = 4\ x$ OR	$Te^- = 4\ (17)(\frac{18}{17}) = 72$
$ON_C = 4\ (1 - \frac{nO_2}{x})$	$ON_C = 4\ (1 - \frac{18}{17}) = -\frac{4}{17}$	$ON_C = 4\ (1 - OR)$	$ON_C = 4\ (1 - \frac{18}{17}) = -\frac{4}{17}$

Example 7. Given Cangrelor, 

, $C_{17}H_{25}O_{12}Cl_2F_3N_5S_2P_3$.

(a) Determining all non-carbon ON and all atomic coefficients.

Atom	C	H	O	Cl	F	N	S	P
ON	–	+1	−2	−1	−1	−3	−2	+5
Atomic coefficient	17	25	12	2	3	5	2	3

(b) Balancing the combustion reaction.

The unbalanced combustion reaction of "$C_{17}H_{25}O_{12}Cl_2F_3N_5S_2P_3 + O_2 \rightarrow 17CO_2 + H_2O + HCl + HF + NH_3 + H_2S + H_3PO_4$" can be set up and balanced as follows:

Using atomic coefficient $n_C = nCO_2$:

$$C_{17}H_{25}O_{12}Cl_2F_3N_5S_2P_3 + O_2 \rightarrow 17CO_2 + H_2O + HCl + HF + NH_3 + H_2S + H_3PO_4$$

Balancing HCl:

$$C_{17}H_{25}O_{12}Cl_2F_3N_5S_2P_3 + O_2 \rightarrow 17CO_2 + H_2O + 2HCl + HF + NH_3 + H_2S + H_3PO_4$$

Balancing HF:

$$C_{17}H_{25}O_{12}Cl_2F_3N_5S_2P_3 + O_2 \rightarrow 17CO_2 + H_2O + 2HCl + 3HF + NH_3 + H_2S + H_3PO_4$$

Balancing NH_3:

$$C_{17}H_{25}O_{12}Cl_2F_3N_5S_2P_3 + O_2 \rightarrow 17CO_2 + H_2O + 2HCl + 3HF + 5NH_3 + H_2S + H_3PO_4$$

Balancing H_2S:

$$C_{17}H_{25}O_{12}Cl_2F_3N_5S_2P_3 + O_2 \rightarrow 17CO_2 + H_2O + 2HCl + 3HF + 5NH_3 + 2H_2S + H_3PO_4$$

Balancing H_3PO_4:

$$C_{17}H_{25}O_{12}Cl_2F_3N_5S_2P_3 + O_2 \rightarrow 17CO_2 + H_2O + 2HCl + 3HF + 5NH_3 + 2H_2S + 3H_3PO_4$$

Balancing H_2O:

$$C_{17}H_{25}O_{12}Cl_2F_3N_5S_2P_3 + O_2 \rightarrow 17CO_2 - 4H_2O + 2HCl + 3HF + 5NH_3 + 2H_2S + 3H_3PO_4$$

$$C_{17}H_{25}O_{12}Cl_2F_3N_5S_2P_3 + O_2 + 4H_2O \rightarrow 17CO_2 + 2HCl + 3HF + 5NH_3 + 2H_2S + 3H_3PO_4$$

Balancing O_2:

$$C_{17}H_{25}O_{12}Cl_2F_3N_5S_2P_3 + 15O_2 + 4H_2O \rightarrow 17CO_2 + 2HCl + 3HF + 5NH_3 + 2H_2S + 3H_3PO_4$$

$nO_2 = 15$	$nCO_2 = 17$	$OR = \frac{15}{17}$

(c) Calculating Te^- and ON_C from nO_2 or OR.

Calculating Te^- and ONc			
From nO_2		From OR	
Mathematical equation	Calculation	Mathematical equation	Calculation
$Te^- = 4\ nO_2$	$Te^- = 4\ (15) = 60$	$Te^- = 4\ \ x\ OR$	$Te^- = 4\ (17)\ (\frac{15}{17}) = 60$
$ON_C = 4\ (1 - \frac{nO_2}{x})$	$ON_C = 4\ (1 - \frac{15}{17}) = +\frac{8}{17}$	$ON_C = 4\ (1 - OR)$	$ON_C = 4\ (1 - \frac{15}{17}) = +\frac{8}{17}$

In Examples 6 and 7, firstly the combustion reactions of $C_xH_yO_zX_wN_vS_uP_t$ molecules are balanced; secondly the nO_2, and nCO_2 can be identified; and thirdly their corresponding Te^- and ON_C can be determined by using nO_2 or OR.

Conclusions

The concepts of ON_C and Te^- play significant roles in both pure and applied chemistry. However, the tasks of assigning ON_C and counting Te^- are challenging. In this article, the interrelationships among nO_2, OR, Te^-, and ON_C are established by using an organic combustion reaction as a model. Consequently, six sets of mathematical equations among these four parameters of organic compounds in the general chemical formula of $C_xH_yO_zX_wN_vS_uP_t$ are formulated. Furthermore, ON_C and Te^- of a given organic compound can be determined by the derived mathematical equations.

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