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## Research article

Pong Kau Yuen\* and Cheng Man Diana Lau

# Application of stoichiometric hydrogen atoms for balancing organic combustion reactions

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**Abstract:** Combustion is a common redox reaction, and organic combustion is one of the basic contents in chemistry curriculum. The transferred H-atom is commonly used as a redox indicator in organic chemistry and biochemistry. Nevertheless, the relationship between the number of transferred H-atoms and the number of transferred electrons has not been fully revealed. Oxidation number (ON) is an electron-counting concept. Without knowing the ONs, the number of transferred electrons cannot be counted and therefore, the redox reactions cannot be classified, defined, and balanced. This paper explores the new H-atom method for counting the number of transferred H-atoms. It provides a half-reaction approach to balance the overall organic combustion reactions. Only simple arithmetic procedures are needed to determine the number of transferred H-atoms and consequently the number of transferred electrons. According to this method, the mathematical formulas for assigning the number of transferred H-atoms can be deduced by balancing the general chemical formulas of organic compounds in half and overall organic combustions. Furthermore, the number of transferred electrons and their stoichiometric categories can be determined conveniently by any given organic chemical formula in organic combustion reactions.

**Keywords:** balancing organic combustion reaction; number of transferred electrons; number of transferred H-atoms; organic combustion; stoichiometry.

## Introduction

Combustion is a common redox reaction, and organic combustion reactions and stoichiometry are some of the basic contents in general chemistry curriculum (Chang & Goldsby, 2013; Tro, 2014). When learning about redox reaction, it is fundamental to understand its classification, definition, and methods of balancing (Goodstein, 1970). Numerous papers discussed the balancing of redox equations (Herndon, 1997; Jensen, 2009; Vitz, 2002). Mathematically the methods can be classified into inspection method (Guo, 1997; Kolb, 1981) and algebraic method (Blakley, 1982; Kolb, 1979; Olson, 1997; Porter, 1985). The nature of redox reaction is an electron transfer reaction. According to IUPAC (2019), the terms of redox reactions can be understood in four different models:  $e^-$  transfer, H-atom transfer, O-atom transfer, and oxidation number (ON) (Table 1).

Students need to know how to count the number of transferred electrons and balance organic combustion reactions. Both the arithmetic and algebraic methods can be applied effectively to balance and deduct a complete combustion equation (Lau & Yuen, 2015). However, they cannot be used to determine the number of transferred electrons. To manage this task, the ON method is more suited. ON is the electron-counting concept

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**Cheng Man Diana Lau**, Macau Chemical Society, Macao, Macao, E-mail: [lauchengman@gmail.com](mailto:lauchengman@gmail.com)

**Table 1:** Terms of redox reactions.

Redox terms	e <sup>-</sup> transfer	H-atom transfer	O-atom transfer	Oxidation number
Oxidation	Loss e <sup>-</sup>	Loss H	Gain O	Increase
Reduction	Gain e <sup>-</sup>	Gain H	Loss O	Decrease

for balancing redox reactions (Fishtik & Berka, 2005; Generalic & Vladislavic, 2018). Nevertheless, many students have difficulty in assigning ON of organic compounds. Up to now, without the knowledge of ONs, the number of transferred electrons cannot be counted; and redox reactions cannot be classified, defined, and balanced. To solve this problem, a new H-atom method is established and developed to count the number of transferred H-atoms without the use of ONs. The H-atom method is based on the loss or gain of hydrogen atoms, and it can be used to determine the number of transferred electrons.

The concept of transferred H-atom is commonly used as a redox indicator in organic chemistry and biochemistry. It has been used for balancing organic half reactions (Chuang, Fedoseev, Ioppolo, van Dishoeck, & Linnartz, 2016; Hayes & Burgess, 2009; Rosado-Reyes, Manion, & Tsang, 2011; Sivaramakrishnan, Michael, Klippenstein, Harding, & Ruscic, 2010). H-atoms can act as reactants (Mutunga, Follett, & Anderson, 2013; Nakamura, Masaki, & Sato, 1985; Paulson, Mutunga, Shelby Follett, & Anderson, 2014); intermediates (Cole-Filipiak, Shapero, Negru, & Neumark, 2014; Dougherty & Rabitz, 1980; Gerasimov & Shatalov, 2013; Simmie, 2003), or products (Beck, Greene, & Ross, 1962; Taylor & Datz, 1955) in chemical reactions. But the relationship between the number of transferred H-atoms and the number of transferred electrons has not been revealed.

This paper explores the new H-atom method for counting the number of transferred H-atoms. The calculation of ON is not needed. The method paves an easy path for balancing organic combustion reactions without losing any chemical relevance. Students simply need to follow straightforward arithmetic procedures to balance half reactions and determine the number of H-atoms, subsequently the number of transferred electrons can be counted.

## Balancing half combustion reactions

In this section, organic compounds, such as hydrocarbons, oxygen-containing hydrocarbons, and halogen-containing hydrocarbons, are used to demonstrate the balancing of half organic combustion reactions. The procedures and examples show how the H-atom method is applied. H-atom, O-atom, and H<sub>2</sub>O act as vehicles for balancing half combustion reactions.

Step 1: Balance all atoms except H and O.

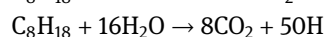
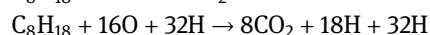
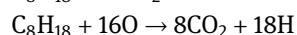
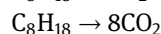
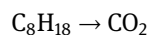
Step 2: Balance oxygen atoms with O.

Step 3: Balance hydrogen atoms with H.

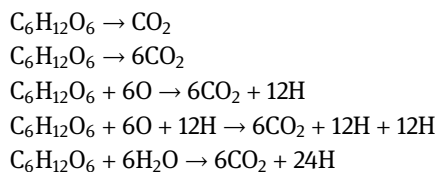
Step 4: Add 2 H atoms for each O atom.

Step 5: Convert 2 H atoms and 1 O atom to 1 H<sub>2</sub>O molecule.

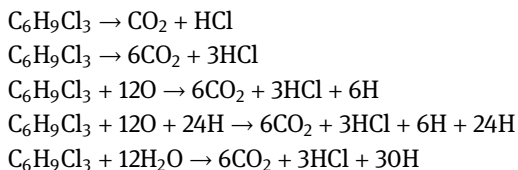
Example 1a: Combustion of hydrocarbon, C<sub>8</sub>H<sub>18</sub>



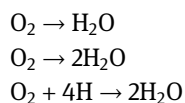
Example 1b: Combustion of oxygen-containing hydrocarbon,  $C_6H_{12}O_6$



Example 1c: Combustion of halogen-containing hydrocarbon,  $C_6H_9Cl_3$



Example 1d: Conversion of  $O_2$  to  $H_2O$



The half combustion reactions and their stoichiometric number of transferred H-atoms are presented in Table 2.

**Table 2:** Stoichiometric number of transferred H-atoms in half combustion reactions.

Half reaction	Number of transferred H-atoms	Type of half reaction
$C_8H_{18} + 16H_2O \rightarrow 8CO_2 + 50H$	Loss of 50H	Oxidation
$C_6H_{12}O_6 + 6H_2O \rightarrow 6CO_2 + 24H$	Loss of 24H	Oxidation
$C_6H_9Cl_3 + 12H_2O \rightarrow 6CO_2 + 3HCl + 30H$	Loss of 30H	Oxidation
$O_2 + 4H \rightarrow 2H_2O$	Gain of 4H	Reduction

## Balancing overall combustion reactions

The following procedures of the H-atom method show how the overall organic combustion reactions are balanced.

Step 1: Divide an overall combustion reaction into two half reactions.

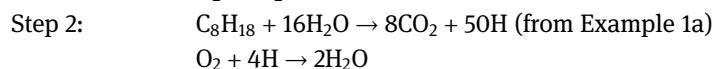
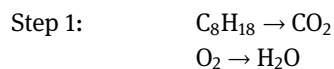
Step 2: Balance all atoms in the two half reactions.

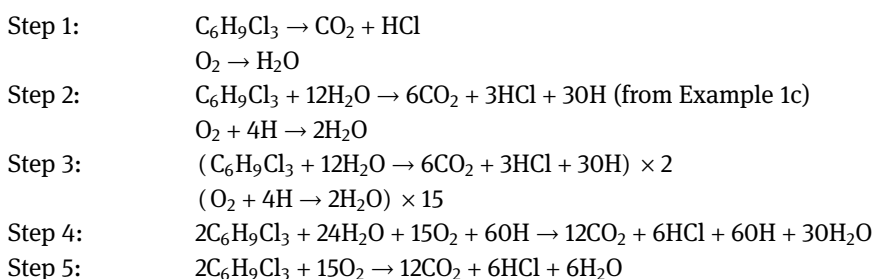
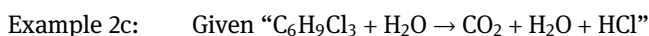
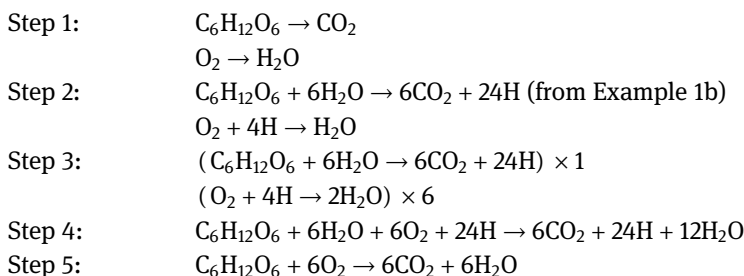
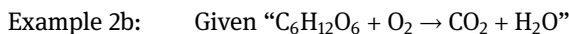
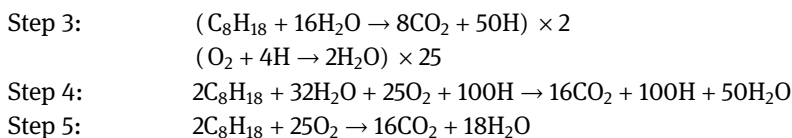
Step 3: Make the H-atom of the two half reactions equivalent.

Step 4: Combine the two half reactions.

Step 5: Simplify the overall chemical equation.

Example 2a: Given " $C_8H_{16} + O_2 \rightarrow CO_2 + H_2O$ "





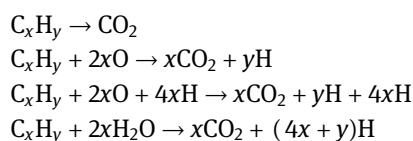
The stoichiometric number of transferred H-atoms in an overall combustion reaction is equal to the LCM of the number of transferred H-atoms in their two half reactions (Table 3).

**Table 3:** Stoichiometric number of transferred H-atom in overall combustion reactions.

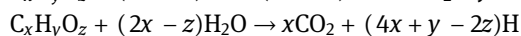
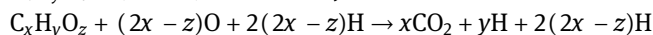
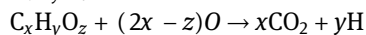
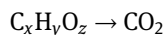
Overall combustion reaction	Stoichiometric number of transferred H-atoms
$2\text{C}_8\text{H}_{18} + 25\text{O}_2 \rightarrow 16\text{CO}_2 + 18\text{H}_2\text{O}$	LCM of (4H) and (50H) = 100H
$\text{C}_6\text{H}_{12}\text{O}_6 + 6\text{O}_2 \rightarrow 6\text{CO}_2 + 6\text{H}_2\text{O}$	LCM of (4H) and (24H) = 24H
$2\text{C}_6\text{H}_9\text{Cl}_3 + 15\text{O}_2 \rightarrow 12\text{CO}_2 + 6\text{HCl} + 6\text{H}_2\text{O}$	LCM of (4H) and (30H) = 60H

## Deducting the general half organic combustion equations

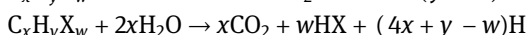
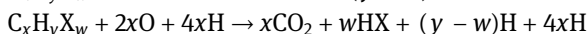
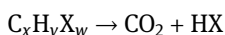
The general half combustion equations for hydrocarbons and their hydrocarbons derivatives can be deducted by the H-atom method. Examples of stoichiometric categories are shown as follows.



Example 3b: Given  $C_xH_yO_z + O_2 \rightarrow CO_2 + H_2O$



Example 3c: Given  $C_xH_yX_w + O_2 \rightarrow CO_2 + H_2O + HX$



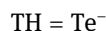
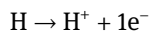
The general half combustion equations and the number of transferred H-atoms are presented in Table 4.

**Table 4:** General half combustion equations and the number of transferred H-atoms.

Half combustion reaction	Number of transferred H-atoms
$C_xH_y + 2xH_2O \rightarrow xCO_2 + (4x + y)H$	$4x + y$
$C_xH_yO_z + (2x - z)H_2O \rightarrow xCO_2 + (4x + y - 2z)H$	$4x + y - 2z$
$C_xH_yX_w + 2xH_2O \rightarrow xCO_2 + wHX + (4x + y - w)H$	$4x + y - w$
$O_2 + 4H \rightarrow 2H_2O$	4

## Determining the number of transferred electrons

The number of transferred H-atoms and transferred electrons are corresponding. The loss of one H-atom equals the loss of one electron, and the gain of one H-atom equals the gain of one electron.



where TH = number of transferred H-atoms

$Te^-$  = number of transferred electrons

TH > 0 (loss of H-atom; oxidation)

TH < 0 (gain of H-atom; reduction)

$Te^- > 0$  (loss of electron; oxidation)

$Te^- < 0$  (gain of electron; reduction)

TH (overall) = LCM of TH (oxidation) and TH (reduction)

$Te^-$  (overall) = LCM of  $Te^-$  (oxidation) and  $Te^-$  (reduction)

The number of transferred H-atoms can be counted by using the general formulas of half combustion reactions, and  $Te^-$  can be determined by the general half combustion equations (Table 5).

**Table 5:** General half combustion equations of TH and  $Te^-$ .

Reactant	General half combustion equation	TH = $Te^-$
$C_xH_y$	$C_xH_y + 2xH_2O \rightarrow xCO_2 + (4x + y)H$	$4x + y$ (oxidation)
$C_xH_yO_z$	$C_xH_yO_z + (2x - z)H_2O \rightarrow xCO_2 + (4x + y - 2z)H$	$4x + y - 2z$ (oxidation)
$C_xH_yX_w$	$C_xH_yX_w + 2xH_2O \rightarrow xCO_2 + wHX + (4x + y - w)H$	$4x + y - w$ (oxidation)
$O_2$	$O_2 + 4H \rightarrow 2H_2O$	4 (reduction)

## Deducting the general overall organic combustion equations

The general combustion equations of hydrocarbons and its hydrocarbons derivatives can be deducted by following the steps below. After deduction, their stoichiometric categories are identified. They demonstrate the number of transferred H-atoms and all participating mole relationships for organic combustion equations.

Example 4a: Given  $C_xH_y + O_2 \rightarrow CO_2 + H_2O$

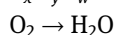
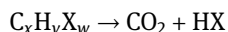
- Step 1: Divide into two half reactions  
 $C_xH_y \rightarrow CO_2$   
 $O_2 \rightarrow H_2O$
- Step 2: Balance all atoms in the two half reactions  
 $C_xH_y + 2xH_2O \rightarrow xCO_2 + (4x + y)H$   
 $O_2 + 4H \rightarrow 2H_2O$
- Step 3: Make the H-atom of the two half reactions equivalent [LCM = 4 and  $(4x + y)$ ]  
 $(C_xH_y + 2xH_2O \rightarrow xCO_2 + (4x + y)H) \times 4$   
 $(O_2 + 4H \rightarrow 2H_2O) \times (4x + y)$
- Step 4: Combine the two half reactions  
 $4C_xH_y + 8xH_2O + (4x + y)O_2 + 4(4x + y)H \rightarrow 4xCO_2 + 4(4x + y)H + 2(4x + y)H_2O$
- Step 5: Simplify the overall chemical equation  
 $4C_xH_y + 8xH_2O + (4x + y)O_2 \rightarrow 4xCO_2 + 2(4x + y)H_2O$   
 $4C_xH_y + (4x + y)O_2 \rightarrow 4xH_2O + 2(4x + y)H_2O - 8xH_2O$   
 $4C_xH_y + (4x + y)O_2 \rightarrow 4xCO_2 + 2yH_2O$   
 $C_xH_y + \frac{4x+y}{4} O_2 \rightarrow xCO_2 + \frac{y}{2} H_2O$

Example 4b: Combustion of  $C_xH_yO_z$ : Given  $C_xH_yO_z + O_2 \rightarrow CO_2 + H_2O$

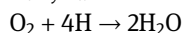
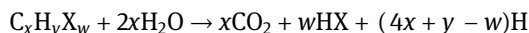
- Step 1: Divide into two half reactions  
 $C_xH_yO_z \rightarrow CO_2$   
 $O_2 \rightarrow H_2O$
- Step 2: Balance all atoms in the two half reactions  
 $C_xH_yO_z + (2x - z)H_2O \rightarrow xCO_2 + (4x + y - 2z)H$   
 $O_2 + 4H \rightarrow 2H_2O$
- Step 3: Make the H-atom of the two half reactions equivalent [LCM = 4 and  $(4x + y - 2z)$ ]  
 $(C_xH_yO_z + (2x - z)H_2O \rightarrow xCO_2 + (4x + y - 2z)H) \times 4$   
 $(O_2 + 4H \rightarrow 2H_2O) \times (4x + y - 2z)$
- Step 4: Combine the two half reactions  
 $4C_xH_yO_z + 4(2x - z)H_2O + (4x + y - 2z)O_2 + 4(4x + y - 2z)H$   
 $\rightarrow 4xCO_2 + 4(4x + y - 2z)H + 2(4x + y - 2z)H_2O$
- Step 5: Simplify the overall chemical equation  
 $4C_xH_yO_z + (4x + y - 2z)O_2 \rightarrow 4xCO_2 + 2(4x + y - 2z)H_2O - 4(2x - z)H_2O$   
 $4C_xH_yO_z + (4x + y - 2z)O_2 \rightarrow 4xCO_2 + 2yH_2O$   
 $4C_xH_yO_z + (4x + y - 2z)O_2 \rightarrow 4xCO_2 + 2yH_2O$   
 $C_xH_yO_z + \frac{4x+y-2z}{4} O_2 \rightarrow xCO_2 + \frac{y}{2} H_2O$

Example 4c: Given  $C_xH_yO_z + O_2 \rightarrow CO_2 + H_2O + HX$

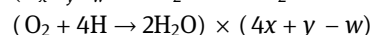
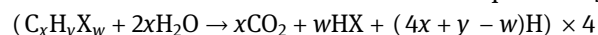
Step 1: Divide into two half reactions



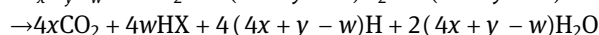
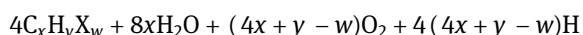
Step 2: Balance all atoms in the two half reactions



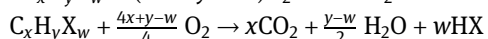
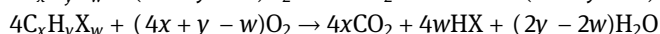
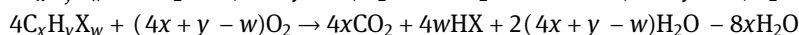
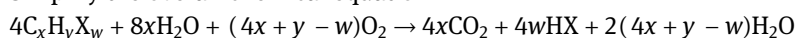
Step 3: Make the H-atom of the two half reactions equivalent [LCM = 4 and  $(4x + y - w)$ ]



Step 4: Combine the two half reactions



Step 5: Simplify the overall chemical equation



The general overall combustion equations, the number of transferred H-atoms, and the number of transferred electrons are shown in Table 6.

**Table 6:** General overall combustion equations and the number of transferred H-atoms.

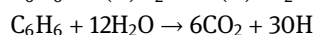
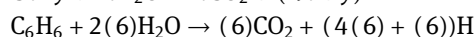
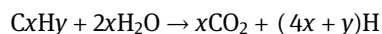
Overall combustion reaction	TH (overall) = $Te^-$ (overall)
$C_xH_y + \frac{4x+y}{4} O_2 \rightarrow xCO_2 + \frac{y}{2} H_2O$	LCM of 4 and $(4x + y)$
$C_xH_yO_z + \frac{4x+y-2z}{4} O_2 \rightarrow xCO_2 + \frac{y}{2} H_2O$	LCM of 4 and $(4x + y - 2z)$
$C_xH_yX_w + \frac{4x+y-w}{4} O_2 \rightarrow xCO_2 + \frac{y-w}{2} H_2O + wHX$	LCM of 4 and $(4x + y - w)$

## Determining $Te^-$ and balancing organic combustion reactions

Based on the general half and overall combustion equations, any given chemical formula of organic compound can reveal its number of transferred electrons and balance its half and overall combustion reactions.

Example 5: Given a hydrocarbon  $C_6H_6$ :  $x = 6$ ;  $y = 6$

(i) balance a half combustion

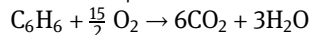
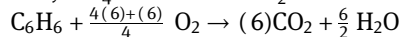
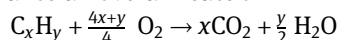


(ii) count  $Te^-$  (oxidation) =  $4x + y$

$$Te^- \text{ (oxidation)} = 4(6) + (6)$$

$$= +30$$

(iii) balance an overall reaction



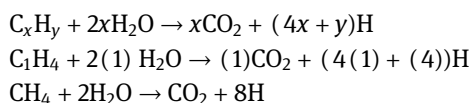


$$\begin{aligned}
 \text{(iv) count Te}^- \text{ (overall)} &= \text{LCM of 4 and } 4x + y \\
 \text{Te}^- \text{ (overall)} &= \text{LCM of 4 and } 4(6) + (6) \\
 &= \text{LCM of 4 and 30} \\
 &= 60
 \end{aligned}$$

By using the general formulas of half and overall organic combustion reactions, an organic compound,  $C_6H_6$ , demonstrates that it loses 30 electrons in the half oxidation reaction and exchanges 60 electrons in the overall combustion reaction. In addition, their stoichiometric categories can be represented in the balanced organic combustion reactions.

Example 6: Given a hydrocarbon  $CH_4$ :  $x = 1$ ;  $y = 4$

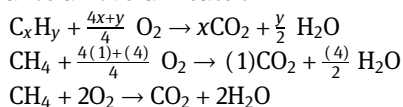
(i) balance a half combustion



(ii) count  $Te^-$  (oxidation) =  $4x + y$

$$\begin{aligned}
 Te^- \text{ (oxidation)} &= 4(1) + (4) \\
 &= +8
 \end{aligned}$$

(iii) balance an overall reaction

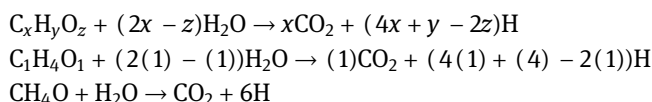


(iv) count  $Te^-$  (overall) = LCM of 4 and  $4x + y$

$$\begin{aligned}
 Te^- \text{ (overall)} &= \text{LCM of 4 and } 4(1) + (4) \\
 &= \text{LCM of 4 and 8} \\
 &= 8
 \end{aligned}$$

Example 7: Given an oxygen-containing hydrocarbon  $CH_3OH$  ( $CH_4O$ ):  $x = 1$ ;  $y = 4$ ;  $z = 1$

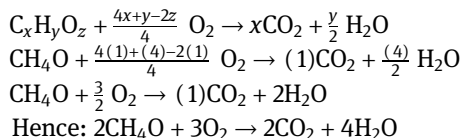
(i) balance a half combustion



(ii) count  $Te^-$  (oxidation) =  $4x + y - z$

$$\begin{aligned}
 Te^- \text{ (oxidation)} &= 4(1) + (4) - 2(1) \\
 &= +6
 \end{aligned}$$

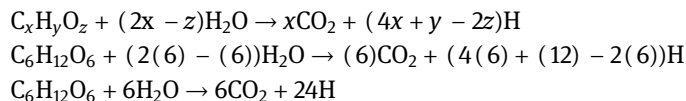
(iii) balance an overall reaction



$$\begin{aligned}
 \text{(iv) count } \text{Te}^- \text{ (overall)} &= \text{LCM of 4 and } 4x + y - 2z \\
 \text{Te}^- \text{ (overall)} &= \text{LCM of 4 and } 4(1) + (4) - 2(1) \\
 &= \text{LCM of 4 and 6} \\
 &= 12
 \end{aligned}$$

Example 8: Given an oxygen-containing hydrocarbon  $\text{C}_6\text{H}_{12}\text{O}_6$ :  $x = 6$ ;  $y = 12$ ;  $z = 6$

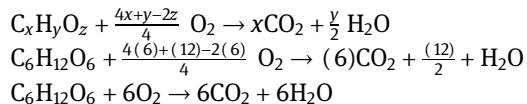
(i) balance a half combustion



(ii) count  $\text{Te}^-$  (oxidation)

$$\begin{aligned}
 \text{C}_x\text{H}_y\text{O}_z + (2x - z)\text{H}_2\text{O} &\rightarrow x\text{CO}_2 + (4x + y - 2z)\text{H} \\
 \text{Te}^- \text{ (oxidation)} &= 4x + y - 2z \\
 \text{Te}^- \text{ (oxidation)} &= 4(6) + (12) - 2(6) \\
 &= +24
 \end{aligned}$$

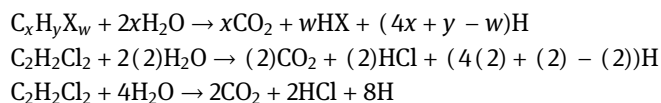
(iii) balance an overall reaction



$$\begin{aligned}
 \text{(iv) count } \text{Te}^- \text{ (overall)} &= \text{LCM of 4 and } 4x + y - 2z \\
 \text{Te}^- \text{ (overall)} &= \text{LCM of 4 and } 4(6) + (12) - 2(6) \\
 &= \text{LCM of 4 and 24} \\
 &= 24
 \end{aligned}$$

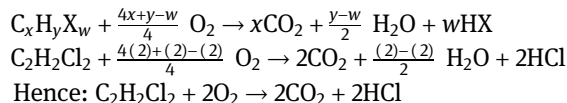
Example 9: Given a halogen-containing hydrocarbon  $\text{C}_2\text{H}_2\text{Cl}_2$ :  $x = 2$ ;  $y = 2$ ;  $w = 2$

(i) balance a half combustion



$$\begin{aligned}
 \text{(ii) count } \text{Te}^- \text{ (oxidation)} &= 4x + y - w \\
 \text{Te}^- \text{ (oxidation)} &= 4(2) + (2) - (2) \\
 &= +8
 \end{aligned}$$

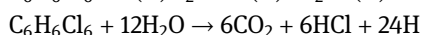
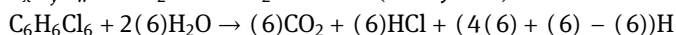
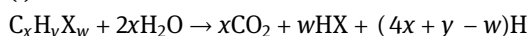
(iii) balance an overall reaction



$$\begin{aligned}
 \text{(iv) count } \text{Te}^- \text{ (overall)} &= \text{LCM of 4 and } 4x + y - w \\
 \text{Te}^- \text{ (overall)} &= \text{LCM of 4 and } 4(2) + (2) - (2) \\
 &= \text{LCM of 4 and 8} \\
 &= 8
 \end{aligned}$$

Example 10: Given a halogen-containing hydrocarbon  $C_6Cl_6$ :  $x = 6$ ;  $y = 0$ ;  $w = 6$

(i) balance a half combustion

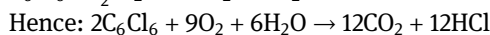
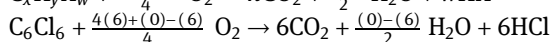
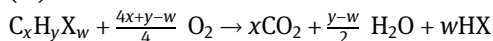


(ii) count  $Te^-$  (oxidation) =  $4x + y - w$

$$Te^- \text{ (oxidation)} = 4(6) + (0) - (6)$$

$$= +18$$

(iii) balance an overall reaction



(iv) count  $Te^-$  (overall) = LCM of 4 and  $4x + y - w$

$$Te^- \text{ (overall)} = \text{LCM of } 4 \text{ and } 4(6) + (0) - (6)$$

$$= \text{LCM of } 4 \text{ and } 18$$

$$= 36$$

## Conclusion

The knowledge of counting the number of transferred electrons and balancing organic combustion reactions is important for chemistry students. Although both the arithmetic and algebraic methods can be applied to balance and deduct a complete combustion equation, they cannot be used to determine the number of transferred electrons. To count the number of transferred electrons, ON has to be known. However, the determination of the ON is not necessarily easy. This paper explores a new H-atom method, which can reveal the number of transferred electrons.

According to this method, the number of transferred H-atoms is used as an electron counting concept instead of the ON. It provides an easy path for balancing organic combustion reactions without losing any chemical relevance. Students simply need to follow straightforward arithmetic procedures to determine the number of transferred H-atoms and subsequently the number of transferred electrons can be counted. The application of the H-atom method is not limited to organic combustion reactions. It works for all H-atom transfer reactions. The mathematical formulas for assigning the number of transferred H-atoms can be known by deducting the general chemical formulas of organic compounds in half and overall organic combustions. Furthermore, the number of transferred electrons and their stoichiometric categories can be determined conveniently by any given organic chemical formula in organic combustion reactions.

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