Combustion Analysis of Organic Compounds: A Special Type of Empirical Formula Problem

Information:

When compounds that contain carbon, hydrogen, and/or oxygen burn in air; carbon dioxide and water are the only reaction products. If a compound with unknown composition is burned, all of the carbon can be found in the carbon dioxide and all of the hydrogen will be found in the water. It is impossible to track the oxygen as some oxygen from air ends up in the products. It is possible to use the conservation of mass to calculate the mass of the oxygen present in the original compound.

Model 1: Tracking the atoms in a combustion reaction

Example of a combustion reaction:

$CH_3COOH + 2\ O_2 \dashrightarrow 2\ CO_2 + 2\ H_2O$

If 1 mole of CH_3COOH is burned in excess oxygen, 2 moles of carbon dioxide and 2 moles of water are produced.

Critical Thinking Questions

1. How many moles of carbon dioxide would be produced from 2 moles of CH_3COOH?

   2 mol $CH_3CO_2H \longrightarrow$ 4 mol CO_2 produced

2. How many moles of oxygen atoms originate from the organic compound if 1 mole of CH_3COOH is burned?

   $\underline{1 \text{ mol } CH_3CO_2H} \quad \frac{N_A \text{ molec.}}{\text{mol}} \quad \frac{2\text{-O-atoms}}{1 \text{ molec}}$

3. If 1 mole of CH_3COOH is burned, what mass of CH_3COOH reacts?

   $\begin{array}{r} 28 \\ 32 \\ \hline 60 \end{array}$

   1 mol × mm(60) = 60g CH_3CO_2H

4. If 1 mole of CH_3COOH is burned, what mass of CO_2 is produced?

   $1 \text{ mol } CH_3CO_2H \times \frac{2 \text{ mol } CO_2}{1 \text{ mol}} \times \frac{44 g\ CO_2}{\text{mol}} = 88\ g\ CO_2$

5. If 1 mole of CH_3COOH is burned, what mass of H_2O is produced?

$$\frac{1 \text{ mol MeOH}}{} \cdot \frac{2 \text{ mol } H_2O}{1 \text{ mol}} \cdot \frac{18 \text{ g } H_2O}{\text{mol}} = 36 \text{ g } H_2O$$

6. Use the Law of Conservation to determine the mass of oxygen reacted.

$$60\text{g MeOH} + ?\text{g } O_2 \longrightarrow 88\text{ g } CO_2 + 36\text{ g } H_2O$$

$124 - 60 = 64\text{ g } O_2$ $\quad$ 124 g

7. Using your results from #4 and #5, determine the moles of hydrogen present in the water produced and the moles of carbon in the carbon dioxide produced.

$$\frac{88\text{ g } CO_2}{} \cdot \frac{\text{mol } CO_2}{44\text{ g}} \cdot \frac{1 \text{ mol C}}{1 \text{ mol } CO_2} = 2 \text{ mol C}$$

$$\frac{36\text{ g } H_2O}{} \cdot \frac{\text{mol } H_2O}{18\text{ g}} \cdot \frac{2 \text{ mol H}}{1 \text{ mol } H_2O} = 4 \text{ mol H}$$

8. Compare your answers to #7 with the chemical formula of the compound being reacted.

$CH_3CO_2H \longrightarrow 2$ mol C & 4 mol H

same

9. If you did not know the formula of the original organic compound, but did know it contained carbon and hydrogen, how could you use information about the moles of carbon dioxide and water formed by the reaction to determine the moles of carbon and hydrogen in the compound?

go backward. assume all C from $C_xH_y \rightarrow CO_2$ & all H $\rightarrow H_2O$

Model 2: Some Combustion Data

A 1.50 g sample of hydrocarbon undergoes complete combustion to produce 4.40 g of CO_2 and 2.70 g of H_2O.

$$C_xH_y + O_2 \longrightarrow CO_2 + H_2O$$

1.50g $\quad$ 4.40g $\quad$ 2.70g

Critical Thinking Questions

10. Why does the total mass of product produced exceed the mass of the hydrocarbon reacted?

need mass O_2

turns into CO_2 turns into H_2O

11. Where did all of the carbon and hydrogen from the original compound end up at the completion of the reaction?

12. Would it be true that the moles of carbon in the carbon dioxide is equal to the moles of carbon in the hydrocarbon? Explain.

yes (b/c mol : mol)

13. Would it be true that the mass of carbon in the carbon dioxide is equal to the mass of carbon in the hydrocarbon? Explain.

no (not g : g)

14. Use the given information to determine the moles of carbon and moles of hydrogen in the carbon dioxide and water produced by the combustion reaction.

$$\frac{4.40\,g\,CO_2}{} \cdot \frac{mol\,CO_2}{44\,g} \cdot \frac{1\,mol\,C}{1\,mol\,CO_2} = 0.1\,mol\,C$$

$$\frac{2.70\,g\,H_2O}{} \cdot \frac{mol\,H_2O}{18\,g} \cdot \frac{2\,mol\,H}{1\,mol\,H_2O} = 0.3\,mol\,H$$

80% C
20% H

15. Determine the empirical formula of the hydrocarbon.

find 1:3 ratio $\longrightarrow$ C_1H_3 (÷ each by smallest)

There are other ways to do this

Model 3: Compounds with oxygen

A 0.2500 g sample of a compound known to contain carbon, hydrogen and oxygen undergoes complete combustion to produce 0.3664 g of CO_2 and 0.1500 g of H_2O. What is the empirical formula of this compound?

$$\underset{0.250g}{C_xH_4O_2} + O_2 \longrightarrow \underset{0.3664g}{CO_2} + \underset{0.1500g}{H_2O}$$

Critical Thinking Questions

16. Use the Law of Conservation to determine the mass of oxygen that reacted from the air.

0.5164 g total P − 0.250 g $C_xH_4O_2$ = 0.2664 g O_2

17. Do the calculations necessary to show that the amount of carbon in the original hydrocarbon is about 0.10 g and the amount of hydrogen in the original compound is about 0.017 g.

$$\frac{0.3664g\ CO_2}{} \cdot \frac{mol\ CO_2}{44g} \cdot \frac{1\ mol\ C}{1\ mol\ CO_2} \times \frac{12g}{mol} = 0.0999\ g\ C$$

$$\frac{0.1500g\ H_2O}{} \cdot \frac{mol\ H_2O}{18g} \cdot \frac{2\ mol\ H}{1\ mol\ H_2O} \cdot \frac{1.01g}{mol} = 0.0168g\ H$$

18. Why does the total mass of carbon and hydrogen not add up to the original mass of the original compound?

missing O

0.250g $C_xH_4O_2$

have 0.1167g C + g H

19. Use the Law of Conservation to determine the mass of oxygen in the original compound.

$$0.250g - 0.1167g = 0.1333g\ O$$

20. Use the data to determine the empirical formula of the compound.

$$0.0999g\ C/12 = 0.00833\ mol\ C/0.00833 = 1$$
$$0.0168g\ H/1 = 0.0168\ mol\ H/0.00833 = 2$$
$$0.1333g\ O/16 = 0.00833\ mol\ O/0.00833 = 1$$
CH_2O

Problem to Try

Quinone, which is used in the dye industry and in photography, is an organic compound containing only C, H, and O. What is the empirical formula of the compound if you find that 0.105 g of the compound gives 0.257 g of CO_2 and 0.0350 g of H_2O when burned completely?

$$C_xH_yO_z + O_2 \longrightarrow CO_2 + H_2O$$
0.105g — 0.257g — 0.0350g

$$\frac{0.257g\ CO_2}{} \cdot \frac{mol\ CO_2}{44g} \cdot \frac{1\ mol\ C}{1\ mol\ CO_2} \cdot \frac{12g\ C}{mol} = 0.070g\ C$$

$$\frac{0.0350g\ H_2O}{} \cdot \frac{mol\ H_2O}{18g} \cdot \frac{2\ mol\ H}{1\ mol\ H_2O} \cdot \frac{1g\ H}{mol} = 0.00389g\ H$$

$$0.105g - 0.070g\ C - 0.00389g\ H = 0.0311g\ O$$

$$0.070g\ C/12 = 0.00583\ mol\ C/0.00194 = 3$$
$$0.00389g\ H/1 = 0.00389\ mol\ H/0.00194 = 2$$
$$0.0311g\ O/16 = 0.00194\ mol\ O/0.00194 = 1$$
C_3H_2O