Combustion Analysis

How can burning a substance help determine the substance's chemical formula?

Why?

Scientists have many techniques to help them determine the chemical formula or structure of an unknown compound. One commonly used technique when working with carbon-containing compounds is combustion analysis. Any compound containing carbon and hydrogen will burn. With an ample oxygen supply, the products of the combustion will be carbon dioxide and water. Analyzing the mass of CO_2 and H_2O that are produced allows chemists to determine the ratios of elements in the compound.

Model 1 – Combustion Reactions

CH_4	+	$2O_2$	→	CO_2	+	$2H_2O$
C_2H_6	+	$\frac{7}{2}O_2$	→	$2CO_2$	+	$3H_2O$
C_2H_4	+	$3O_2$	→	$2CO_2$	+	$2H_2O$
C_3H_8	+	$5O_2$	→	$3CO_2$	+	$4H_2O$

1. According to Model 1, what reactant is always required for combustion?

   Oxygen is always required for combustion.

2. Balance the reactions in Model 1 while keeping the hydrocarbon coefficient a "1." This may require the use of fractions in other places.

   See Model 1.

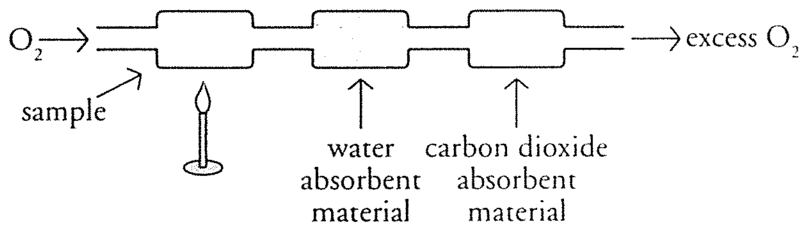
3. How is the coefficient of CO_2 in the chemical reactions in Model 1 related to the chemical formula of the hydrocarbon being analyzed?

   The coefficient of CO_2 is the same as the subscript on the carbon atoms in the hydrocarbon.

4. How is the coefficient of the H_2O in the chemical reactions in Model 1 related to the chemical formula of the hydrocarbon being analyzed?

   STOP *The coefficient of H_2O is half the subscript on the hydrogen in the hydrocarbon.*

Read This!



In a combustion analysis experiment, a hydrocarbon sample is heated in a stream of oxygen gas. As the sample burns, water and carbon dioxide is pushed through a series of chambers with materials that absorb each of the respective products. The chambers are each weighed before and after the combustion to determine the mass of each product.

Model 2 – Combustion Analysis of C_xH_y Unknowns

10.00-g Sample	Mass of CO_2 Produced	Moles of CO_2	Moles of Carbon Atoms	Mass of H_2O Produced	Moles of H_2O	Moles of Hydrogen Atoms	Sample's Empirical Formula	Total Mass of C and H Atoms
1	27.42 g	*0.623*	*0.623*	22.46 g	*1.247*	*2.493*	CH_4	*10.00 g*
2	29.26 g	*0.665*	*0.665*	17.97 g	*0.997*	*1.994*	CH_3	*10.00 g*

30.00-g Sample	Mass of CO_2 Produced	Moles of CO_2	Moles of Carbon Atoms	Mass of H_2O Produced	Moles of H_2O	Moles of Hydrogen Atoms	Sample's Empirical Formula	Total Mass of C and H Atoms
3	94.11 g	*2.139*	*2.139*	38.53 g	*2.139*	*4.277*	CH_2	*30.00 g*
4	89.80 g	*2.041*	*2.041*	49.03 g	*2.721*	*5.442*	C_3H_8	*30.00 g*

5. Discuss with your group how the data in Model 2 could be used to calculate the following quantities:

   Moles of CO_2 Moles of C atoms

   Moles of H_2O Moles of H atoms

   Divide the work among group members to complete those four columns in Model 2. Show work for your calculations below.

$$27.42\ g\ CO_2 \times \frac{1\ mole}{44.01\ g} = 0.6232\ mole\ CO_2 \rightarrow 0.6232\ mole\ C\ atoms$$

$$22.46\ g\ H_2O \times \frac{1\ mole}{18.016\ g} = 1.247\ moles\ H_2O \rightarrow 2.493\ moles\ H\ atoms$$

STOP

6. Discuss with your group how the data from Model 2 could be used to find the lowest whole number ratio between carbon and hydrogen atoms. This will give you the empirical formulas of the sample substances. Fill in the last column of Model 2.

   0.6232 mole C : 2.493 mole H $\rightarrow$ *1 : 4* $\rightarrow$ CH_4

7. Did you need balanced chemical combustion equations to find the empirical formulas of the unknowns in Model 2?

   No, balanced chemical equations were not needed.

8. Did you need to know the mass of the samples to find the empirical formulas of the unknowns in Model 2?

   No, the mass of the samples was not needed.

9. What other information would you need to determine the molecular formulas?

   To find the molecular formulas, you would need to know the molar mass of the unknown compounds.

10. A 15.00-g sample of an unknown hydrocarbon is analyzed by combustion analysis. The sample produced 50.70 grams of carbon dioxide and 10.42 grams of water. Find the empirical formula of the unknown.

$$50.70\ g\ CO_2 \times \frac{1\ mole}{44.00\ g} = 1.153\ moles\ CO_2 \rightarrow 1.152\ moles\ C\ atoms$$

$$10.42\ g\ H_2O \times \frac{1\ mole}{18.016\ g} = 0.5783\ mole\ H_2O \rightarrow 1.157\ moles\ H\ atoms$$

STOP

1.152 mole C : 1.157 mole H $\rightarrow$ *1 : 1* $\rightarrow$ *CH*

11. Calculate the total mass of carbon atoms and hydrogen atoms for each sample in Model 2. Divide the work among group members. Create a new column in Model 2 for these data.

    a. How does the mass of carbon and hydrogen atoms compare to the mass of the original sample?

    The total mass of carbon and hydrogen atoms is equal to the original sample mass.

    b. Name the scientific law that justifies your answer to part *a*.

    The law of conservation of mass.

    c. Would part *a* be true if the original sample included atoms other than carbon and hydrogen? For example: C_2H_6O or $C_2H_5NH_2$. Justify your reasoning.

    If other elements were in the sample, the total mass of carbon and hydrogen atoms would be less than the mass of the sample. The nitrogen or oxygen atoms would be missing from the mass.

Read This!

When the combustion analysis unknown is a compound containing only carbon and hydrogen, all of the atoms in the sample end up in either the CO_2 or H_2O products. However, if the unknown contains other elements, like oxygen or nitrogen, those atoms might end up in the CO_2 and H_2O products (in the case of oxygen) or they might form other gases that move through the apparatus without being captured. Additionally, O atoms may come from the atmosphere as opposed to the combusting sample. Moles of these atoms cannot be calculated by stoichiometry directly. Instead, we must use the law of conservation of mass.

Model 3 – Combustion Analysis of $C_xH_yO_z$ Unknowns (10.00-g samples)

Sample	Mass of CO_2 Produced	Moles of Carbon Atoms	Mass of H_2O Produced	Moles of Hydrogen Atoms	Total Mass of C and H Atoms	Mass of O Atoms	Moles of O Atoms	Sample's Empirical Formula
1	19.10 g	*0.4341*	11.73 g	*1.302*	*6.526*	*3.47*	*0.217*	C_2H_6O
2	14.65 g	*0.3330*	6.00 g	*0.6661*	*4.6621*	*5.34*	*0.333*	CH_2O
3	21.96 g	*0.4991*	11.99 g	*1.331*	*7.325*	*2.67*	*0.167*	C_3H_8O
4	28.05 g	*0.6375*	5.74 g	*0.637*	*8.287*	*1.713*	*0.107*	C_6H_6O

12. Four unknown hydrocarbons containing oxygen were analyzed by combustion analysis. The samples were 10.00 g each. The results are shown in Model 3. Discuss with your group what calculations would need to be performed to complete the table in Model 3. Divide the work among group members. Show work for your calculations below.

$$19.10\ g\ CO_2 \times \frac{1\ mole}{44.00\ g} = 0.4341\ mole\ CO_2 \rightarrow 0.4341\ mole\ C\ atoms \rightarrow 5.214\ g\ carbon$$

$$11.73\ g\ H_2O \times \frac{1\ mole}{18.016\ g} = 0.6511\ mole\ H_2O \rightarrow 1.302\ moles\ H\ atoms \rightarrow 1.312\ g\ hydrogen$$

$$Total\ mass\ of\ C\ and\ H\ atoms = 6.526\ g$$

$$Mass\ of\ O\ atoms = 10.00\ g - 6.526\ g = 3.47\ g\ oxygen$$

$$3.47\ g\ O \times \frac{1\ mole}{15.999\ g} = 0.217\ mole\ O$$

$$\frac{0.4341\ mole}{0.217\ mole} : \frac{1.302\ moles}{0.217\ mole} : \frac{0.217\ mole}{0.217\ mole} \rightarrow 2C : 6H : 1O$$

STOP

13. Did you need balanced chemical combustion equations to find the empirical formula of your unknowns in Model 3?

No, a balanced chemical equation was not needed.

14. Did you need to know the mass of the samples to find the empirical formulas of your unknowns in Model 3?

Yes, the total mass of the samples was needed to find the mass of oxygen atoms.

15. A 15.00-g sample of a compound containing carbon, hydrogen and nitrogen is analyzed by combustion analysis. The sample produced 29.3 grams of carbon dioxide and 20.8 grams of water. Find the empirical formula of the unknown.

$$29.3\ g\ CO_2 \times \frac{1\ mole}{44.00\ g} = 0.666\ mole\ CO_2 \rightarrow 0.666\ mole\ C\ atoms \rightarrow 8.00\ g\ carbon$$

$$20.8\ g\ H_2O \times \frac{1\ mole}{18.016\ g} = 1.15\ moles\ H_2O \rightarrow 2.31\ moles\ H\ atoms \rightarrow 2.31\ g\ hydrogen$$

Total mass of C and H atoms $= 10.31\ g$

Mass of N atoms $= 15.00\ g - 10.31\ g = 4.69\ g$ *nitrogen*

$$4.69\ g\ N \times \frac{1\ mole}{14.01\ g} = 0.335\ mole\ N$$

C_2H_7N

STOP

Extension Questions

16. It is critical in combustion analysis procedures that the sample be dry. Discuss what errors in data would occur if the sample contained moisture. How might this affect the final empirical formula?

    If the sample contains water impurities, then the water would evaporate from the sample during combustion and be absorbed by the water absorbent material. The mass of water would be too high, making the moles of hydrogen too high. The calculated empirical formula would have too many hydrogen atoms.

17. Discuss what errors in data would occur if the sample contained a carbon-based impurity. How might this affect the final empirical formula?

    If the sample contains a carbon impurity, then the carbon would burn just like the carbon in the sample, creating too much CO_2. This would lead to calculating too many moles of carbon. The calculated empirical formula would have too many carbon atoms.

18. Balance the general combustion equation below *using variables* for the missing coefficients.

$$C_xH_y + \frac{y}{4}O_2 \rightarrow xCO_2 + \frac{y}{2}H_2O$$