Chapter 3

Empirical formula & Combustion Analysis

PERCENT COMPOSITION

- ***The percent composition is the mass percentage of each type of atom(element) in a compound.***

$$\%X = \left(\frac{\text{total atomic mass of X}}{\text{molar mass which contains X}} \right) 100$$

For Example:

Calculate the percent composition of nicotine, $C_{10}H_{14}N_2$.

- **Molar mass nicotine = 10C + 14H + 2N = 162 g/mol**

$$\%C = \left(\frac{10\ C}{C_{10}H_{14}N_2} \right) 100 = \left(\frac{120\ g/mol}{162\ g/mol} \right) 100 = 74.1\%$$

$$\%H = \left(\frac{14\ H}{C_{10}H_{14}N_2} \right) 100 = \left(\frac{14\ g/mol}{162\ g/mol} \right) 100 = 8.64\%$$

$$\%N = \left(\frac{2\ N}{C_{10}H_{14}N_2} \right) 100 = \left(\frac{28\ g/mol}{162\ g/mol} \right) 100 = 17.3\%$$

PERCENT COMPOSITION

Q. How many grams of lithium will combine with 20.0 g of sulfur to form Li_2S?

Molar mass of Li_2S = 2Li + S = 46 g/mol

1. **Calculate the % of Li in Li_2S = 2(6.94g/mol)/46g/mol = 30.4%**
2. **Calculate the % of S in Li_2S = 100% - 30.4% = 69.6%**
3. **A ratio can now be established:**

$$\frac{20.0\text{ g S}}{?\text{ g Li}} = \frac{69.6\%}{30.4\%} \qquad ? = \frac{(30.4\%)\,(20.0\text{ g})}{69.6\%} \qquad x = 8.74\text{ g}$$

PERCENT COMPOSITION

- ***The percent composition can also be calculated from experimental data.***

A student prepares a compound of tungsten chloride from 3.946 g of tungsten and 3.806 g of chlorine. *Assuming the reaction goes to completion*, **calculate the percent composition.**

$$W + Cl_2 \rightarrow W_xCl_y$$

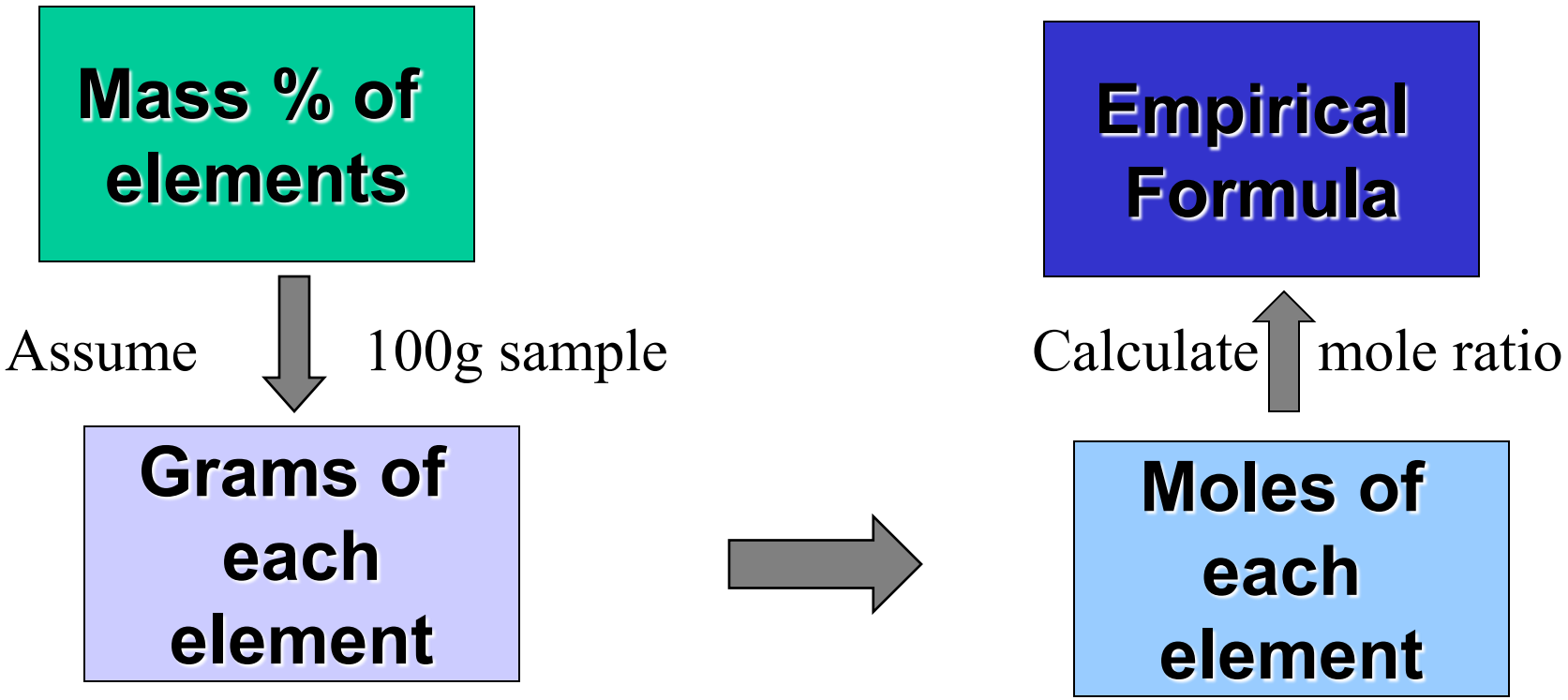
According to the LCM, 3.946 g of W combines with 3.806 g of Cl to give 7.752 g of compound.

$$\%W = \left(\frac{\text{mass W}}{\text{mass } W_xCl_y}\right)100 = \left(\frac{3.946\text{ g}}{7.752\text{ g}}\right)100 = 50.9\%$$

50.9% W &
49.1% Cl

$$\%Cl = \left(\frac{\text{mass Cl}}{W_xCl_y}\right)100 = \left(\frac{3.806\text{ g}}{7.752\text{ g}}\right)100 = 49.1\%$$

EMPIRICAL FORMULA



EMPIRICAL FORMULA

Step 1: If given the % composition, assume a 100g sample then convert % to grams.

Step 2: Use the atomic masses to convert grams to moles.

Step 3: Divide the moles of each element by the SMALLEST mole fraction.

Step 4: The results from step 3 should be a whole number, if not, make it so by multiplying by a common factor.

Determining Empirical Formulas

1) The compound **para**-aminobenzoic acid (you may have seen it listed as PABA on your bottle of sunscreen) is composed of carbon (61.31%), hydrogen (5.14%), nitrogen (10.21%), and oxygen (23.33%). Find the empirical formula of PABA.

- Allow for 100.00 g of **para**-aminobenzoic acid and converting to moles:

$$\text{C}: 61.31\,\text{g} \times \frac{1\,\text{mol}}{12.01\,\text{g}} = 5.105\ \text{mol C}$$

$$\text{H}: 5.14\,\text{g} \times \frac{1\,\text{mol}}{1.01\,\text{g}} = 5.09\ \text{mol H}$$

$$\text{N}: 10.21\,\text{g} \times \frac{1\,\text{mol}}{14.01\,\text{g}} = 0.7288\ \text{mol N}$$

$$\text{O}: 23.33\,\text{g} \times \frac{1\,\text{mol}}{16.00\,\text{g}} = 1.456\ \text{mol O}$$

Determining Empirical Formulas

- Calculate the mole ratio by dividing by the smallest number of moles:

$$\text{C: } \frac{5.105 \text{ mol}}{0.7288 \text{ mol}} = 7.005 \approx 7$$

$$\text{H: } \frac{5.09 \text{ mol}}{0.7288 \text{ mol}} = 6.984 \approx 7$$

$$\text{N: } \frac{0.7288 \text{ mol}}{0.7288 \text{ mol}} = 1.000$$

$$\text{O: } \frac{1.458 \text{ mol}}{0.7288 \text{ mol}} = 2.001 \approx 2$$

- These are the subscripts for the empirical formula:

$C_7H_7NO_2$

Empirical Formula

Hydroquinone, used as a photographic developer, is 65.4% carbon, 5.5% hydrogen, and 29.1% oxygen by mass. What is the empirical formula of hydroquinone?

Step 1: make it 100g sample
Step 2: convert g → mol using molar mass
Step 3: Choose smallest value to divide by

65.7% → 65.7 g C $\left(\frac{1 \text{ mole}}{12.011 \text{ g/mol}}\right)$ = 5.46998 moles C
5.5% → 5.5 g H $\left(\frac{1 \text{ mole}}{1.008 \text{ g/mol}}\right)$ = 5.5 moles H
29.1% → 29.1 g O $\left(\frac{1 \text{ mole}}{16.00 \text{ g/mol}}\right)$ = 1.81875 moles O

5.46998 / 1.81875 = 3 C 5.5 / 1.81875 = 3 H

Empirical Formula = C_3H_3O

Molecular Formula

Adipic acid is used in the manufacture of nylon. The percent composition of the acid is 49.3% carbon, 6.9% hydrogen, and 43.8% oxygen by mass. The molecular weight of the compound is 146 g/mol. What is the molecular formula?

$49.3\% \rightarrow 49.3\text{ g C}\ \left(\frac{1\text{ mole}}{12.011\text{ g/mol}}\right) = 4.10457\text{ moles C}$

$6.9\% \rightarrow 6.9\text{ g H}\ \left(\frac{1\text{ mole}}{1.008\text{ g/mol}}\right) = 6.84523\text{ moles H}$

$43.8\% \rightarrow 43.8\text{ g O}\ \left(\frac{1\text{ mole}}{16.00\text{ g/mol}}\right) = 2.73750\text{ moles O}$

$4.10457 / 2.73750 = 1.5\text{ C}$ $\qquad$ $6.84523 / 2.73750 = 2.5\text{ H}$

Need whole number so multiple by 2

$2(1.5) = 3\text{ C}$ & $2(2.5) = 5\text{ H}$

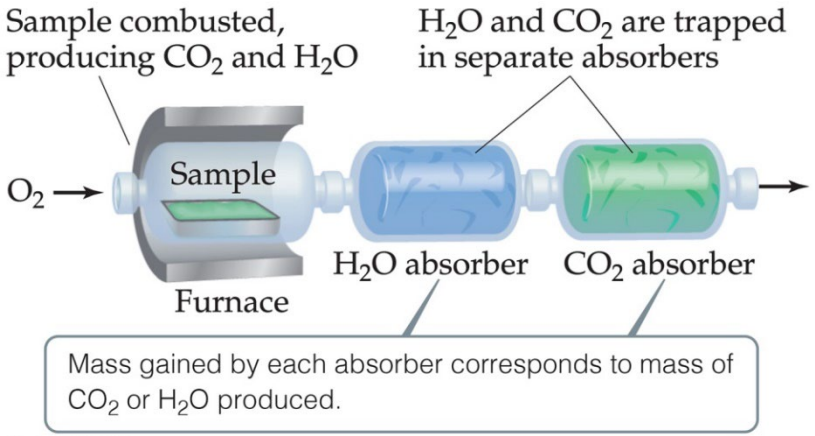
Empirical Formula = $C_3H_5O_2$

Next: molar mass/ Empirical mass = multiplier for empirical formula

(146 g/mol) / (73 g/mol) = 2

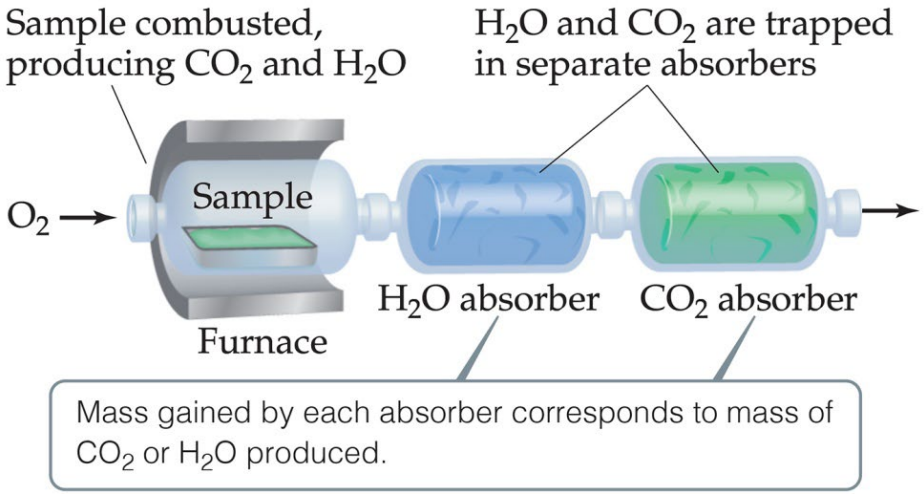
Molecular Formula = $C_6H_{10}O_4$

Combustion Analysis (1 of 3)

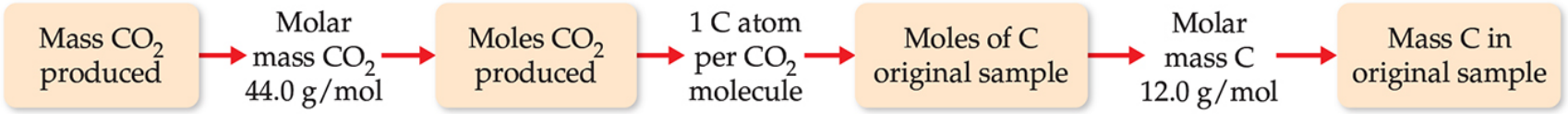


- Compounds containing C, H, and O are routinely analyzed through combustion in a chamber.
  - Mass of C is determined from the mass of C O_2 produced.
  - Mass of H is determined from the mass of H_2O produced.
  - Mass of O is determined by the difference of the mass of the compound used and the total mass of C and H.
  - Note: The mass of O in the compound can NOT be determined from CO_2 and H_2O because oxygen is added during the combustion.

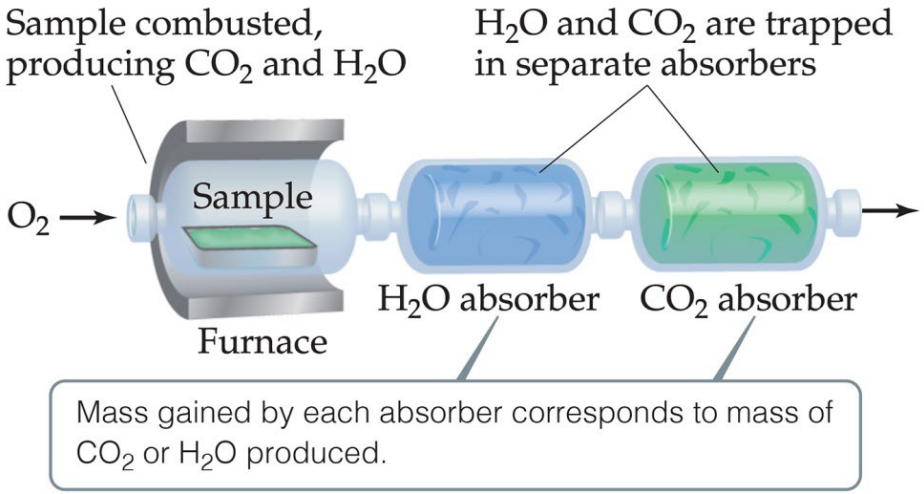
Combustion Analysis (2 of 3)



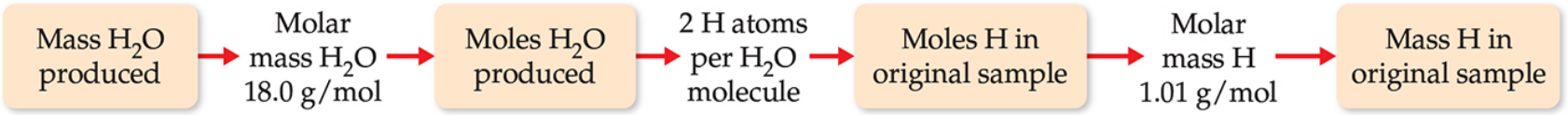
- Mass of C is determined from the mass of CO_2 produced.



Combustion Analysis (3 of 3)



- Mass of H is determined from the mass of H_2O produced.



Empirical Formula - Combustion Analysis

Menthol (MM = 156.3 g/mol), a strong smelling substance used in cough drops, is a compound of carbon, hydrogen, and oxygen. When 0.1595 g of menthol was subjected to combustion analysis, it produced 0.449 g of CO_2 and 0.184 g of water. What is its molecular formula?

$$C_xH_yO_z + O_2 \rightarrow CO_2 + H_2O$$

0.1595 g 0.4735g 0.449g 0.184g

0.449g CO_2 ($^{1\ mole}/_{44\ g/mol}$)= 0.010205 mol ($^{1mol\ C}/_{1mol\ CO_2}$)= 0.010205 mol C

0.449g CO_2 ($^{1\ mole}/_{44\ g/mol}$)= 0.010205 mol ($^{2mol\ O}/_{1mol\ CO_2}$)= 0.020410 mol O

0.184g H_2O ($^{1\ mole}/_{18\ g/mol}$) = 0.010222 mol ($^{1mol\ O}/_{1mol\ H_2O}$)= 0.010222 mol O

0.184g H_2O ($^{1\ mole}/_{18\ g/mol}$) = 0.010222 mol ($^{2mol\ H}/_{1mol\ H_2O}$)= 0.020444 mol H

We need to combine the oxygen's on the product side & then subtract the excess oxygen NOT in the menthol!

0.4735 g O ($^{1\ mole}/_{16.00\ g/mol}$) = 0.02959 moles of excess O from O_2

Total product oxygen – excess oxygen from O_2 = oxygen in compound

(0.020410 + 0.010222) – 0.02959 = 0.001042 mol O

Empirical Formula - Combustion Analysis

Menthol (MM = 156.3 g/mol), a strong smelling substance used in cough drops, is a compound of carbon, hydrogen, and oxygen. When 0.1595 g of menthol was subjected to combustion analysis, it produced 0.449 g of CO_2 and 0.184 g of water. What is its molecular formula?

$$C_xH_yO_z + O_2 \rightarrow CO_2 + H_2O$$

0.1595 g 0.4735g 0.449g 0.184g

0.010205 mol C / 0.001042 mol C = 9.8 C

0.020444 mol H / 0.001042 mol H = 19.6 H

0.001042 mol O / 0.001042 mol O = 1 O

Pick the smallest & divide

Empirical Formula = $C_{10}H_{20}O$

it has a molar mass of 156 g/mol so this is also the molecular formula

SELF-STUDY QUIZ

1. **A 5.325-g sample of methyl benzoate, a compound used in the manufacture of perfumes, is found to contain 3.758 g of C, 0.316 g of H, and 1.251 g of O. What is the empirical formula of this substance?**

2. **A compound contains only carbon, hydrogen, and oxygen. Combustion of 10.68 mg of the compound yields 16.01 mg of CO_2 and 4.37 mg of H_2O. The molar mass of the compound is 176.1 g/mol. What are the empirical and molecular formulas of the compound?**