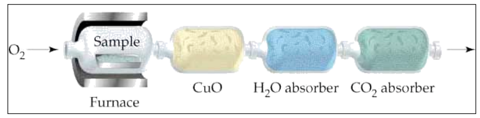
Molecular Formula Calculations
Combustion & Weight Percent

- $C_xH_y + (x + y/4)\ O_2 \rightarrow x\ CO_2 + y/2\ H_2O$
- $C_2H_5OH + 3\ O_2 \rightarrow 2\ CO_2 + 3\ H_2O$

Combustion Analysis

- $C_xH_y + O_2 \rightarrow x\ CO_2 + y/2\ H_2O$



$$C_xH_y + \left(x + \frac{y}{4}\right) O_{2\,(g)} \rightarrow x\ CO_{2(g)} + \frac{y}{2}\ H_2O_{(g)}$$

Combustion Problem

Problem: Erythrose (*MM* = 120.0 g/mol) is an important chemical compound in chemical synthesis.

It contains Carbon, Hydrogen and Oxygen. Combustion analysis of a 700.0 mg sample yielded 1.027 g CO_2 and 0.4194 g H_2O.

Erythrose Solution

Mass fraction of **C** in CO_2 = $\dfrac{\text{mol C } x \text{ MM of C}}{\text{mass of 1 mol } CO_2}$ =

= $\dfrac{\text{1 mol C } x \text{ 12.01 g C/ 1 mol C}}{44.01 \text{ g } CO_2}$ = 0.2729 g C / 1 g CO_2

Mass fraction of **H** in H_2O = $\dfrac{\text{mol H } x \text{ MM of H}}{\text{mass of 1 mol } H_2O}$ =

= $\dfrac{\textbf{2 mol H } x \text{ 1.008 g H / } \textbf{1 mol H}}{18.02 \text{ g } H_2O}$ = 0.1119 g H / 1 g H_2O

Calculating masses of C and H:

Mass of Element = mass of compound *x* mass fraction of element

Erythrose Solution

Mass (g) of C = 1.027 g CO_2 *x* $\dfrac{0.2729 \text{ g C}}{1 \text{ g } CO_2}$ = 0.2803 g C

Mass (g) of H = 0.4194 g H_2O *x* $\dfrac{0.1119 \text{ g H}}{1 \text{ g } H_2O}$ = 0.04693 g H

Calculating the mass of O:

Mass (g) of O = Sample mass -(mass of C + mass of H)

= 0.700 g - 0.2803 g C - 0.04693 g H = 0.37277 g O

Calculating moles of each element:

C = 0.2803 g C / 12.01 g C/ mol C = 0.02334 mol C

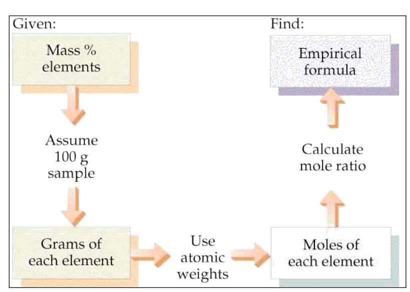
H = 0.04693 g H / 1.008 g H / mol H = 0.04656 mol H

O = 0.37277 g O / 16.00 g O / mol O = 0.02330 mol O

$C_{0.02334}H_{0.04656}O_{0.02330}$ = CH_2O formula weight = 30 g / formula

120 g /mol / 30 g / formula = 4 formula units / cmpd = $\mathbf{C_4H_8O_4}$

Empirical Formulas from Analyses



Empirical Formula Determination

- 1. Use percent analysis.
  Let 100 % = 100 grams of compound.
- 2. Determine the moles of each element.
  (Element % = grams of element.)
- 3. Divide each value of moles by the smallest of the mole values.
- 4. Multiply each number by an integer to obtain all whole numbers.

Empirical & Molecular Formula Determination

Quinine:

C 74.05%, H 7.46%, N 8.63%, O 9.86%

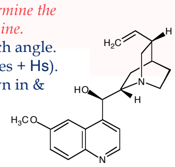
74.05/12.01, 7.46/1.008, 8.63/14.01, 9.86/16.00

$C_{6.166}\ H_{7.40}\ N_{0.616}\ O_{0.616}$

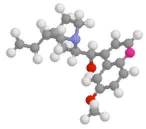
- **Empirical Formula: $C_{10}\ H_{12}\ N_{1}\ O_{1}$**
  Empirical Formula Weight = ?
  Molecular Weight = 324.42
  Molecular Formula = 2x empirical formula
- **Molecular Formula = $C_{20}\ H_{24}\ N_{2}\ O_{2}$**

http://www.3dchem.com/molecules.asp?ID=102

From the structures, determine the molecular formula of quinine.
A Carbon atom is at each angle.
Each C has 4 bonds (lines + Hs).
Hs are not always drawn in & must be added.



C = 20
H = 24
N = 2
O = 2



$C_{20}H_{24}N_2O_2$