Percent Composition of Compounds

- Sometimes, it is helpful or necessary to know a compound's composition in terms of the masses of its elements.
- We can also deduce a molecular formula based on a given percent composition.
- Example:
  - Water is 11.2% hydrogen and 88.8% oxygen. What is the formula for water?

We'll come back to this one....

We can use mass fraction and mass percent to calculate, for example, the composition of this box of marbles...

3 yellow marbles, each weighing 1.0 g
2 purple marbles, each weighing 2.0 g
3 red marbles, each weighing 3.0 g
Total weight = 16.0 g

Mass Fraction and Mass %

Mass fraction = $\frac{\text{mass of one component (element, particle, etc.)}}{\text{total mass (of molecule, box of marbles, etc.)}}$

Calculate the Percent Composition of Sulfuric Acid H_2SO_4

Calculating Mass Percentage and Masses of Elements in a Sample of a Compound

Problem: Sucrose ($C_{12}H_{22}O_{11}$) is common table sugar.
(a) What is the mass percent of each element in sucrose?
(b) How many grams of carbon are in 24.35 g of sucrose?

Empirical and Molecular Formulas

Empirical Formula - The simplest formula for a compound that agrees with the elemental analysis! The smallest set of whole numbers of atoms.

Molecular Formula - The formula of the compound as it really exists. It must be a **multiple** of the empirical formula.

Some Compounds with Empirical Formula CH_2O

(Composition by Mass 40.0% C, 6.71% H, 53.3% O)

Name	Molecular Formula	Whole-Number Multiple	M (g/mol)	Use or Function
Formaldehyde	CH_2O	1	30.03	Disinfectant; biological preservative
Acetic acid	$C_2H_4O_2$	2	60.05	Acetate polymers; vinegar (5% solution)
Lactic acid	$C_3H_6O_3$	3	90.08	Causes milk to sour; forms in muscle during exercise
Erythrose	$C_4H_8O_4$	4	120.10	Forms during sugar metabolism
Ribose	$C_5H_{10}O_5$	5	150.13	Component of many nucleic acids and vitamin B_2
Glucose	$C_6H_{12}O_6$	6	180.16	Major nutrient for energy in cells

Elemental Analysis

Decomposition or combustion analysis is used to determine the mass of each type of element present in a compound.

Figure 3.5:
Schematic Diagram of a Combustion Analysis Device

Determining Empirical Formulas from Measured Masses of Elements - I

The elemental analysis of a sample gave the following results: 5.677g Na, 6.420 g Cr, and 7.902 g O. What is the empirical formula and name of the compound?

Determining Empirical Formulas from Masses of Elements - II

Constructing the preliminary formula:

$Na_{0.5447}Cr_{0.1235}O_{0.4939}$

Converting to integer subscripts:
(dividing all by smallest subscript)

$Na_{1.999}Cr_{1.000}O_{3.999}$

Rounding off to whole numbers:

Na_2CrO_4 sodium chromate

This is the empirical formula...without the molar mass you don't know if it's Na_2CrO_4 or $Na_2Cr_2O_8$ or $Na_{100}Cr_{50}O_{200}$!

Determining the Molecular Formula from Elemental Composition and Molar Mass - I

The sugar burned for energy in cells of the body is glucose (MM = 180.16 g/mol), elemental analysis shows that it contains

40.00 mass % C, 6.729 mass % H, and 53.27 mass % O.

(a) Determine the empirical formula of glucose.
(b) Determine the molecular formula of glucose.

Ascorbic acid (Vitamin C) - I (contains only C , H , and O)

Upon combustion in excess oxygen, a 6.49 mg sample yielded 9.74 mg CO_2 and 2.64 mg H_2O.
Calculate the empirical formula of ascorbic acid.