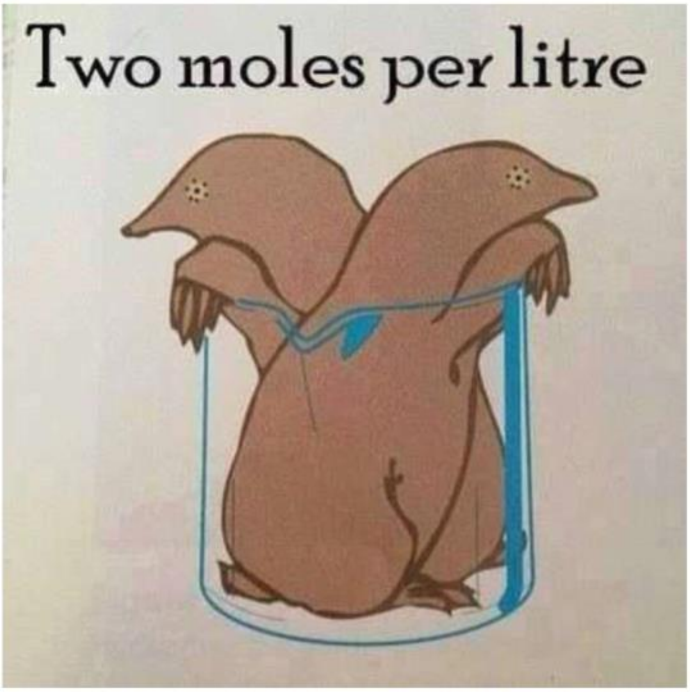
Chemistry 11

Book 2 : Formulae, Hydrates & Complex Dilutions



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Composition Analysis — Determining Formulas

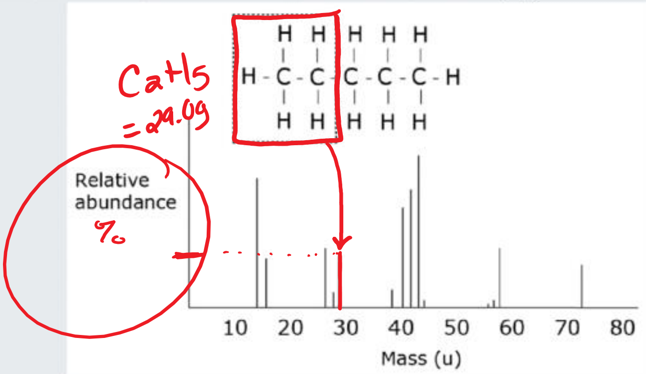
Composition Analysis — Determining Formulas

Fun Facts:

Forensic investigators collect samples from crime scenes. How do technicians identify the unknown samples? An instrument called a **mass spectrometer** can identify the vast majority of compounds. Each compound has a unique mass spectrum; much like each person has a unique fingerprint. A mass spectrometer breaks most of the molecules into fragments. In so doing, it creates a variety of particles from individual atoms to the intact molecule itself, and then marks the mass of each of these particles along a graph's horizontal axis. **The height of the line in the spectrum indicates the relative abundance of that particle.**

how much?

Below is a simplified mass spectrum of a compound called pentane (C_5H_{12}).



Mass spectrum analysis of pentane

Percentage Composition

Percent Composition is the percentage of a compounds mass contributed by each type of atom that makes up that compound.

A compound's percentage composition can be determined theoretically from its formula

EXAMPLE: What is the percentage composition of CH_4? methane

Assume there is 1 mol of the compound. molar mass = 16.0g

total mass of C in compound = $1 \times 12.0g = 12.0g$

total mass of H in compound = $4 \times 1.0g = 4.0g$

$$\frac{\text{mass of C}}{\text{molar mass of comp.}} = \quad \% \text{ of C in compound} = \frac{12.0g}{16.0g} \times 100 = 75.0\%$$

3 s.f.

$$\% \text{ of H in compound} = \frac{4.0g}{16.0g} \times 100 = 25\%$$

2 s.f.

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Sample Problem — Determining Percentage Composition

What is the percentage composition of a sugar with the formula $C_{12}H_{22}O_{11}$?

* assume 1 mol of the compound ⇒ can use molar mass

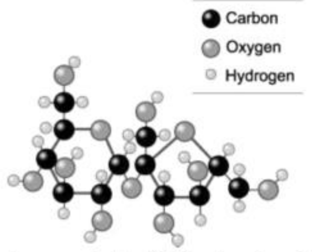
What to Think about	How to Do It
1. Calculate the sugar's molar mass.	Total mass of C = $12 \times (12.0g) = 144.0g$
2. Thus one mole of this sugar contains 144	Total mass of H = $22 \times (1.0g) = 22.0g$

1. Calculate the sugar's molar mass.

Total mass of C = 12 × (12.0g) = 144.0g
Total mass of H = 22 × (1.0g) = 22.0g
Total mass of O = 11 × (16.0g) = 176.0g
molar mass of comp. 342.0g of $C_{12}H_{22}O_{11}$

2. Thus one mole of this sugar contains 144 g C, 22 g H, and 176 g O.

3. Express each element's percentage of the molar mass.



A sugar molecule with 12 carbon atoms, 22 hydrogen atoms, and 11 oxygen atoms.

$$\% C = \frac{144.0g}{342.0g} \times 100 = 42.10\%$$

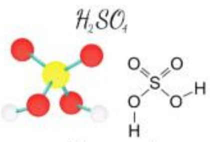
$$\% H = \frac{22.0g}{342.0g} \times 100 = 6.43\%$$

$$\% O = \frac{176.0g}{342.0g} \times 100 = 51.46\%$$

PERCENT COMPOSITION =

$$\frac{\text{(TOTAL MASS OF ELEMENT PRESENT)}}{\text{(MOLECULAR MASS)}} \times 100$$

EXAMPLE: What is the percentage composition of H_2SO_4?



Assume there is 1 mol of the compound. molar mass = 98.1g

total mass of H in compound = 2 × 1.0g = 2.0g

total mass of S in compound = 1 × 32.1g = 32.1g

total mass of O in compound = 4 × 16.0g = 64.0g

molar mass

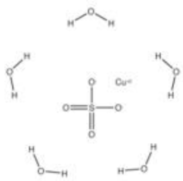
% of H in compound = $\frac{2.0g}{98.1g} \times 100 = 2.0\%$ H

% of S in compound = $\frac{32.1g}{98.1g} \times 100 = 32.7\%$ S

% of O in compound = $\frac{64.0g}{98.1g} \times 100 = 65.2\%$ O

EXAMPLE: What is the percentage of water in $CuSO_4 \cdot 5H_2O$?

whole molecule



Assume there is 1 mol of the compound. molar mass = 249.6g

total mass of H_2O in compound = 5 × 18.0g = 90.0g

16 + 1 + 1 = 18.0

% of H_2O in molecule = $\frac{90.0g \text{ of } H_2O}{249.6g \text{ of } CuSO_4 \cdot 5H_2O} \times 100 = \boxed{36.1\% \ H_2O}$

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ASSIGNMENT #8: Exercises #44-45 (every 2nd letter)

Complete ALL assignments on a **seperate piece of paper** and attach to your booklet when handing in at the end of the unit.

EXERCISES:

44. Calculate the percentage composition of the following.

(a) C_2H_6	(d) $C_2H_4O_2$	(g) $CaCl_2 \cdot 2H_2O$	(j) $C_{17}H_{15}N_3O_2Cl$	(m) $C_2H_4N_2O_4$
(b) $FeCl_2$	(e) $CaCO_3$	(h) $(NH_4)_3PO_4$	(k) $Sn(SO_4)_2 \cdot 2H_2O$	(n) $K_3Fe(CN)_6$
(c) $FeCl_3$	(f) NaOH	(i) $Ag(NH_3)_2Cl$	(l) $(NH_4)_2Sn(OH)_6$	

45. Calculate the percentage of the bold species in each of the following.

(a) $CaCl_2 \cdot 2\mathbf{H_2O}$	(c) $Ce_2(C_2O_4)_3 \cdot 9\mathbf{H_2O}$	(e) $Cr(\mathbf{NH_3})_6Cl_3 \cdot H_2O$	(g) $Cu(\mathbf{C_2H_3O_2})_2 \cdot 2NH_3$
(b) $NiSO_4 \cdot 7\mathbf{H_2O}$	(d) $Al_2(SO_4)_3 \cdot 18\mathbf{H_2O}$	(f) $Cr(NH_3)_6Cl_3 \cdot \mathbf{H_2O}$	(h) $Fe_2(\mathbf{SO_4})_3 \cdot 9H_2O$

12. Calculate the percentage of the bold species in each of the following:

(a) $CaCl_2 \cdot 2\mathbf{H_2O}$ (c) $Ce_2(C_2O_4)_3 \cdot 9\mathbf{H_2O}$ (e) $Cr(\mathbf{NH_3})_6Cl_3 \cdot H_2O$ (g) $Cu(\mathbf{C_2H_3O_2})_2 \cdot 2NH_3$

(b) $NiSO_4 \cdot 7\mathbf{H_2O}$ (d) $Al_2(SO_4)_3 \cdot 18\mathbf{H_2O}$ (f) $Cr(NH_3)_6Cl_3 \cdot \mathbf{H_2O}$ (h) $Fe_2(\mathbf{SO_4})_3 \cdot 9H_2O$

Empirical, Molecular, and Structural Formulas

Every molecular compound has three formulas; an **empirical formula**, a **molecular formula,** and a **structural formula**.

- The **empirical formula** is the simplest ratio of the different types of atoms in the compound.
- * The **molecular formula** is the actual number of each type of atom in each molecule of the compound.
- The **structural formula** shows how the atoms in a molecule are arranged. It is a diagram that shows the pattern of the atoms' connections.

Glucose is an organic compound with a molecular formula of ~~$C_6H_{12}O_6$~~. $C_6H_{12}O_6$ (actual # of atoms)
The subscripts 6, 12, 6 can be reduced (simplified) to 1, 2, 1
We don't show the number 1 as a subscript in a formula so the **empirical formula of glucose is** CH_2O ← This formula is NOT glucose (simple ratio)
simplified form

Many compounds have the same empirical formula but ***different molecular formulas****. Their molecular formulas all reduce to the same ratio. For example, all alkenes such as ethene (C_2H_4), propene (C_3H_6), and butene (C_4H_8), have an empirical formula of CH_2 because each of their molecular formulas can be reduced to a 1 to 2 ratio.*

Quick Check

1. Complete the following table.

(actual # of atoms) (simple ratio) *

Structural Formula	Molecular Formula	Empirical Formula
H O I ‖ H - C - C - O - H I H	$C_2H_4O_2$ $\xrightarrow{\div 2}$	CH_2O
O O ‖ ‖ H - O - C - C - O - H	$C_2H_2O_4$ $\xrightarrow{\div 2}$	CHO_2

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The **EMPIRICAL FORMULA** is sometimes called the **SIMPLEST FORMULA** and is the smallest whole-number ratio of atoms which represents the molecular composition of a species. must be a whole number (no decimals or fractions)

EXAMPLE: All of CH_2 , C_2H_4 , C_3H_6 , C_4H_8 and C_5H_{10} contain twice as many H's as C's and therefore the empirical formula (the simplest ratio) for all these molecules is $\mathbf{CH_2}$.

Finding the empirical formula is essentially the opposite procedure to determining the percentage composition of a compound.

Determining an Empirical Formula from Percent Composition

1 ***EXAMPLE:*** **What is the empirical formula of a compound consisting of 80.0% C and 20.0% H?**

Note that neither the chemical formula nor molar mass is known.
Assume you have 100 g of the compound, so that:
That way % = mass (g)

mass of C = 80.0 % of 100 g = 80.0g
mass of H = 20.0 % of 100 g = 20.0g

Use the masses of each element present to determine the number of moles of each element. The mole ratio will determine the Empirical Formula (simplest ratio)

$$\text{moles of C} = 80.0\cancel{g} \times \frac{1\text{ mol}}{12.0\cancel{g}} = 6.67\text{ mol C}$$

$$\text{moles of H} = 20.0\cancel{g} \times \frac{1\text{ mol}}{1.0\cancel{g}} = 20\text{ mol H}$$

Since "100 g" was an arbitrary (but convenient) mass, the numbers of moles calculated have no real significance.

moles of H = 20.0 ~~g~~ x $\frac{1 \text{ mol}}{1.0 \cancel{g}}$ = 20 mol H

Since "100 g" was an arbitrary (but convenient) mass, the numbers of moles calculated have no real significance. However, the **RATIO** which exists between the numbers of moles ***is*** significant.

To find the smallest whole–number ratio, divide both by the **SMALLER** number

moles of C = 6.67 mol ÷ 6.67 = 1

moles of H = 20 mol ÷ 6.67 = 2.998 ≅ 3

According to these "simplest ratio" values, you can now say that carbon and hydrogen atoms are present in the ratio:

C : H
1 : 3 → Empirical Formula CH_3

and the simplest way to express the chemical formula is:

Sample Problem — Determining an Empirical Formula

Determine the empirical formula of a compound that is 48.65% carbon, 8.11% hydrogen, and 43.24% oxygen.

What to Think about *ASSUME* % → g	How to Do It mass → moles
1. In 100.0 g of the substance, there would be 48.65 g C, 8.11 g H, and 43.24 g O. Convert these amounts into moles.	mass C = 48.65g × $\frac{1 \text{mol}}{12.0 \text{g}}$ = 4.0542 mol C mass H = 8.11g × $\frac{1 \text{mol}}{1.0 \text{g}}$ = 8.1100 mol H mass O = 43.24g × $\frac{1 \text{mol}}{16.0 \text{g}}$ = 2.7025 mol O smallest #
2. Divide each molar quantity by the smallest one and then multiply by whatever factor is necessary to find their integral ratio (as shown in a conventional formula). The mole ratio and the individual atom ratio are of course the same. This means the subscripts in a formula can be read either as mole ratios or as individual atom ratios. If this compound has 3 mol of carbon atoms for every 2 mol of oxygen atoms then it has 3 dozen carbon atoms for every 2 dozen oxygen atoms, and 3 carbon atoms for every 2 oxygen atoms.	4.0542 mol C ÷ 2.7025 ⟹ 1.5 C ×2 8.1100 mol H ⟹ 3 H 2.7025 mol O ⟹ 1 O Empirical formula $2 \times (C_{1.5}H_3O_1)$ $\boxed{C_3H_6O_2}$

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IMPORTANT: You must be able to recognize the following fractions and their decimal equivalents.

0.20 = 1/5	0.40 = 2/5	0.67 = 2/3
0.25 = 1/4	0.50 = 1/2	0.75 = 3/4
0.33 = 1/3	0.60 = 3/5	0.80 = 4/5

*Always multiply the ratio to "clear" fractions or decimals

SNEAKY TRICK: You don't have to re–write fractions such as 2.67 in the form 8/3. All you have to do is to recognize that numbers such as 2.67, 1.33, 5.67 and 3.33 involve **THIRDS** and simply multiply the fraction by 3 to clear the fraction. Similarly, numbers like 1.75, 2.25 and 3.75 involve **QUARTERS**, so that multiplying by 4 will clear such fractions.

IMPORTANT

INCREDIBLY, VITALLY IMPORTANT NOTE:

Always carry out calculations to 3 or 4 digits and NEVER round off intermediate values. The numbers 3.60, 3.67, 3.75 and 3.80 are very close to one another and improper round–off of calculations will cause you to multiply by the wrong number when trying to "clear fractions".

EXAMPLE: **What is the empirical formula of a compound containing 81.8% C and 18.2% H?**

* Assume 100.0 g of the compound is taken.

mass of C = 81.8g mass of H = 18.2g

(multiply by 3 to 'clear' fraction)

moles C = 81.8 g × $\frac{1 \text{mol}}{12.0 \text{g}}$ = $\boxed{6.8167}$ mol (smallest #) | ÷6.8167 → 1 | ×3 = 3 C

moles H = 18.2 g × $\frac{1 \text{mol}}{1.0 \text{g}}$ = 18.2 mol | 2.6699 ≅ 2.67 | ×3 = 8 H

Therefore the empirical formula is C_3H_8

Therefore the empirical formula is C_3H_8

ASSIGNMENT #9: Practice Problems #1-3 & Exercises #46 (every 2nd letter) or 3rd letter
Complete ALL assignments on a **seperate piece of paper** and attach to your booklet when handing in at the end of the unit.

Practice Problems — Determining an Empirical Formula

1. A compound is 18.7% Li, 16.3% C, and 65.5% O. Determine its empirical formula.
2. A compound is 9.93% C, 58.6% Cl, and 31.4% F. Determine its empirical formula.
3. A sample of a compound contains 5.723 g Ag, 0.852 g S, and 1.695 g O. Determine its empirical formula.

EXERCISE:

46. Find the empirical formula for the following compounds.
(a) 15.9% B, 84.1% F
(b) 87.5% Si, 12.5% H
(c) 43.7% P, 56.3% O
(d) 77.9% I, 22.1% O
(e) 77.7% Fe, 22.3% O
(f) 70.0% Fe, 30.0% O
(g) 72.4% Fe, 27.6% O
(h) 46.3% Li, 53.7% O
(i) 24.4% C, 3.39% H, 72.2% Cl
(j) 26.6% K, 35.4% Cr, 38.0% O
(k) 21.8% Mg, 27.9% P, 50.3% O
(l) 3.66% H, 37.8% P, 58.4% O
(m) 46.2% C, 7.69% H, 46.2% O
(n) 50.5% C, 5.26% H, 44.2% N

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