Tishk International University
Faculty of Applied Science
Department of Nutrition & Dietetics
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General Chemistry/ NUT 106

Stoichiometry of Formulas & Equations
2nd Lecture

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Objectives

- Mole - Mass Relationships in Chemical Systems
- Determining the Formula of an Unknown Compound
- Writing and Balancing Chemical Equations
- Calculating the Amounts of Reactant and Product
- Calculating Limiting Reagent & Theoretical Yield
- Fundamentals of Solution Stoichiometry

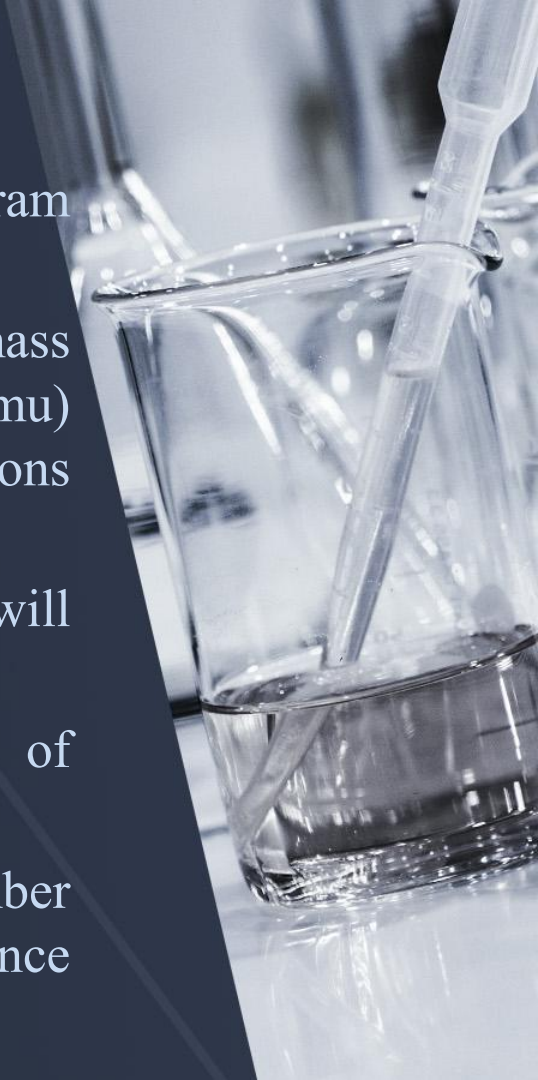
Stoichiometry

Stoichiometry – *The study of the quantitative relationships between elements, compounds, chemical formulas, and chemical reactions.*

- Mass of a substance relative to the chemical entities (atoms, ions, molecules, formula units) comprising the mass.
- Compound – Substance composed of a unique combination of two or more elements.
- Each element in a compound has a unique atomic mass (total mass of protons & neutrons).
- The concept of the "MOLE" was developed to relate the number of entities in a substance to the mass values we determine in the laboratory.
- From the relationship between the number of atoms and the mass of a substance, we can quantify the relationship between elements and compounds in chemical reactions.

Mass vs. Amount

- The standard unit of mass in the metric system is the gram (or kilogram).
- Each of the 100 or so different elements has a unique mass (atomic weight) expressed as either atomic mass units (amu) or grams determined by the number of protons and neutrons in the nucleus.
- The same mass (weight) of two different substances will represent a different number of atoms.
- A chemical equation defines the relative number of molecules of each component involved in the reaction
- The “Mole” establishes the relationship between the number of atoms of a given element and the mass of the substance used in a reaction.



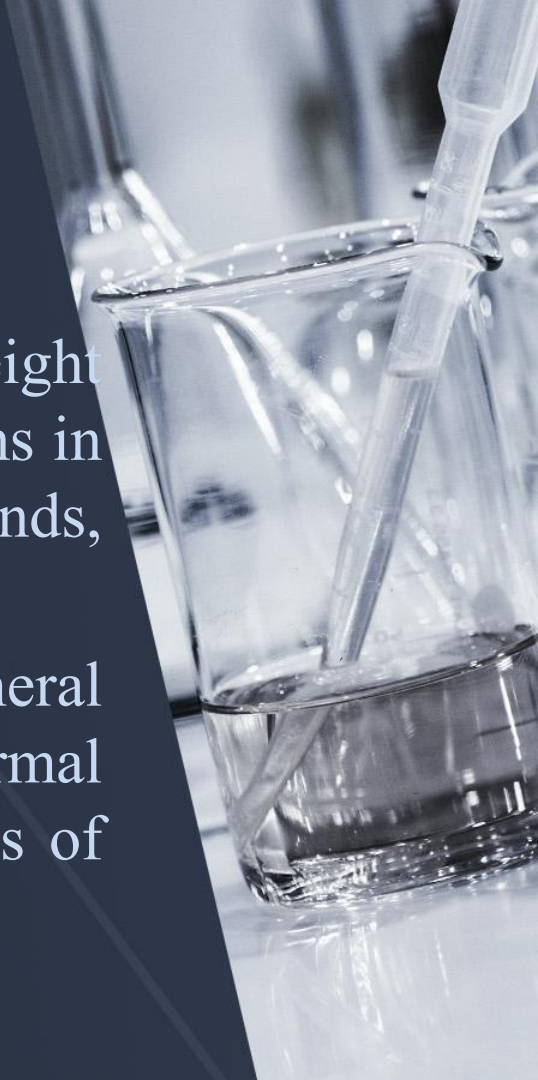
Mass vs. Amount

- Amounts in chemistry are expressed by the mole.
- mole – quantity of substance that contains the same number of molecules or formula units as exactly 12 g of Carbon-12
- Number of atoms in 12 g of Carbon-12 is Avogadro's number (N_A) which equals 6.022×10^{23}.
- The atomic mass of one atom expressed in atomic mass units (amu) is numerically the same as the mass of 1 mole of the element expressed in grams:
- Molar Mass = mass of 1 mole of substance
- One molecule of Carbon (C) has an atomic mass of 12.0107 amu and a molar mass of 12.0107 g/mol
- 1 mole of Carbon contains 6.022×10^{23} atoms
- 1 mole of Sodium contains 6.022×10^{23} atoms

Molecular & Formula Weight

Molecular Mass (also referred to as Molecular Weight (MW) is the sum of the atomic weights of all atoms in a covalently bonded molecule – organic compounds, oxides, etc.

Formula Mass is sometimes used in a more general sense to include Molecular Mass, but its formal definition refers to the sum of the atomic weights of the atoms in ionic bonded compounds.



Molecular & Formula Weight

The computation of Molecular (covalent) or Formula (ionic) molar masses are mathematically the same.

Ex.

Molecular Molar Mass of Methane (CH_4) (covalent bonds)

1 mol CH_4 = 1 mol C/mol CH_4 x 12.0107 g/mol C = 12.0107 g

4 mol H/mol CH_4 x 1.00794 g/mol H = 4.0318 g

= 16.0425 g/mol CH4 = 6.022×10^{23} molecules

Formula Molar Mass of Aluminum Phosphate ($AlPO_4$) (ionic bonds)

1 mol $AlPO_4$ = 1 mol Al/mol $AlPO_4$ x 26.982 g/mol Al) = 26.982

1 mol P/mol $AlPO_4$ x 30.974 g/mol P = 30.974

4 mol O/mol $AlPO_4$ x 15.9994 g/mol O) = 64.000

= 121.954 g/mol $AlPO_4$ = 6.022×10^{23} molecules

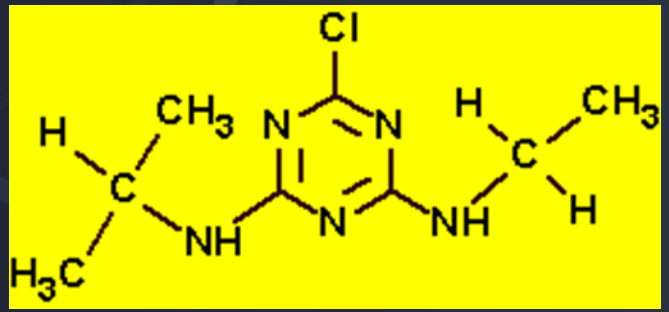
The Concept of Amount

- Summary of Mass Terminology

Isotopic Mass	**Mass of an isotope of an element in atomic mass units (amu)**
Atomic Mass (atomic weight)	Average of the masses of the naturally occurring isotopes of an element based on relative abundance **1 amu =1.66054 x 10^{-24} g** **Atomic Mass Oxygen (O) = 15.9994 amu** **Mass (O)=15.9994 amu x 1.66054 x 10^{-24} g/amu** **=2.65676 x 10^{-23}g**
Molecular Mass Formula Mass	Sum of the atomic masses of the atoms or ions in a molecule or formula unit
Mole	Quantity of substance that contains the same number of molecules or formula units as exactly 12 g of Carbon-12 – 6.022 x 10^{23} molecules
Molar Mass	Mass of 1 mole (6.022 x 10^{23} molecules) of a chemical entity (gram-molecular weight) atom, ion, molecule, formula unit

Mole and Formula Unit

- The widely applied herbicide Atrazine has the following molecular formula
- $C_8H_{14}ClN_5$ Atrazine



$C_8H_{14}ClN_5$ Atrazine

1 mol Atrazine = 6.022×10^{23} molecules

1 mol Atrazine = 8 mol C atoms = $8 \times 6.022 \times 10^{23}$ molecules C

1 mol Atrazine = 14 mol H atoms = $14 \times 6.022 \times 10^{23}$ molecules H

1 mol Atrazine = 1 mol Cl atoms = $1 \times 6.022 \times 10^{23}$ molecules Cl

1 mol Atrazine = 5 mol N atoms = $5 \times 6.022 \times 10^{23}$ molecules N

1 mol Atrazine = 8+14+1+5 = 28 total moles of atoms

Quantities in Chemical Reactions:

- Molecular Weight: sum of atomic weights in molecule of substance (units of amu).
- Formula Weight: sum of atomic weights in formula unit of compound (units of amu).
- Mole (mol): quantity of substance that contains equal numbers of molecules or formula units as in the number of atoms in 12 g of C-12
- Avogadro's number (N_A): 6.022×10^{23}
- Molar Mass: mass of one mole of substance (units of g/mol).

Mole Relationships: Example Calculations

Q/ How many molecules of H_2O are in 251 kg of water?

251 kg x (1000 g/kg) = 2.51×10^5 g H_2O

2.51×10^5 g H_2O x (1 mol H_2O/18.0153 g) = 1.39326×10^4 mol H_2O

1.39326×10^4 mol x 6.022×10^{23} molecules/mol = 8.39021×10^{27} molecules

How many total atoms are in 251 kg of water?

8.39021×10^{27} molecules x (3 atoms/1 molecule) = 2.52×10^{28} atoms

Practice Problems

Q/ What is the molar mass of Caffeine, $C_8H_{10}N_4O_2$?

C=12.0107 g/mol H = 1.00794 g/mol

N=14.0067 g/mol O = 15.9994 g/mol

12.0107 g/mol C x 8 mol C/mol $C_8H_{10}N_4O_2$ = 96.0856 g/mol $C_8H_{10}N_4O_2$

1.00794 g/mol H x 10 mol H/mol $C_8H_{10}N_4O_2$ = 10.0794 g/mol $C_8H_{10}N_4O_2$

14.0067 g/mol N x 4 mol N/mol $C_8H_{10}N_4O_2$ = 56.0268 g/mol $C_8H_{10}N_4O_2$

15.9994 g/mol O x 2 mol O/mol $C_8H_{10}N_4O_2$ = 31.9988 g/mol $C_8H_{10}N_4O_2$

Sum of elemental masses = molecular mass of Caffeine

96.0856 + 10.0794 + 56.0268 + 31.9988 = 194.1906 g/mol $C_8H_{10}N_4O_2$

Practice Problem

How many Sulfur atoms are in 25 g of Al_2S_3?

Al = 26.9815 g/mol S = 32.065 g/mol

Al_2S_3 = 26.98915 g/mol Al x 2 mol Al + 32.065 g/mol S x 3 mol S

= 150.158 g/mol Al_2S_3

25 g Al_2S_3 / 150.158 g/mol Al_2S_3 = 0.166491 mol Al_2S_3

Compute moles of Sulfur atoms

0.166491 mol Al_2S_3 x 3 mol S/1mol Al_2S_3 = 0.499474 mol S atoms

Compute atoms of Sulfur

0.499474 mol S atoms x 6.022 x 10^{23} S atoms/1mol S atoms =

3.008 x 10^{23} atoms S

Percent Composition

It is often necessary to determine the mass percentage of a component in a mixture or an element in a compound.

$$\text{Mass \% A} = \frac{\text{Mass of A in Whole}}{\text{Mass of Whole}} \times 100$$

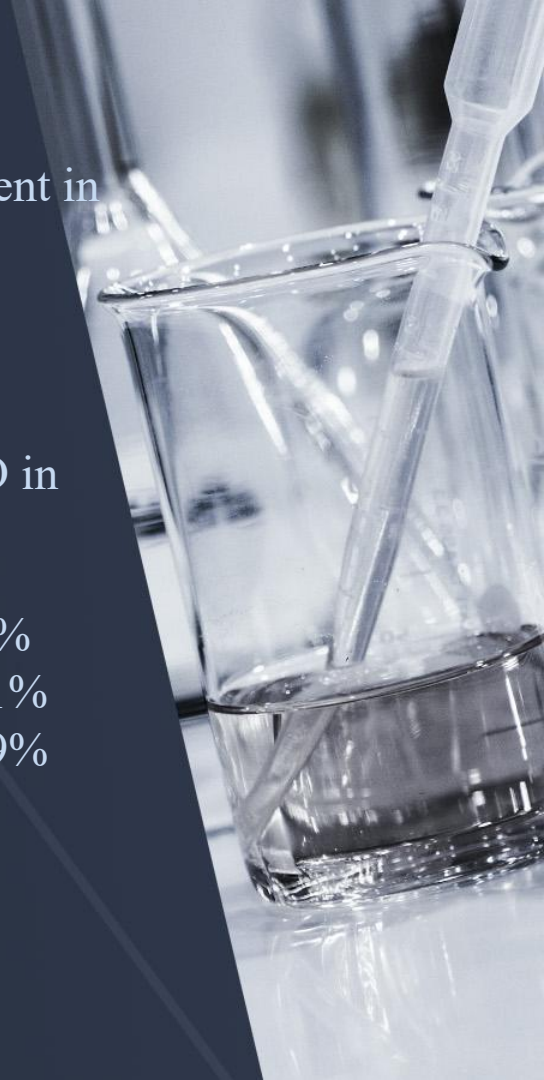
Example calculation: What are the mass percentages of C, H and O in $C_2H_4O_2$ (Acetic Acid)?

1 mol acetic acid = 60.052 g

% C= [2 mol C x (12.0107 g/mol C)] / 60.052 g/mol x 100 = 40.00%

% H = [4 mol H x (1.00794 g/mol C)] / 60.052 g/mol x 100 = 6.71%

% O = [2 mol O x (15.9994 g/mol C)] / 60.052 g/mol x 100 = 53.29%



Practice Problem

Q/ What is the mass percentage of C in in l-Carvone, $C_{10}H_{14}O$, which is the principal component of spearmint?

C = 12.0107 g/mol H = 1.00794 g.mol O = 15.9994 g/mol

a. 30% b. 40% c. 60% d. 70% e. 80%

Ans: e

Molar Mass C = 12.0170 g/mol C x 10 mol C = 120.170 g C

H = 1.00794 g/mol H x 14 mol H = 14.1112 g H

O = 15.9994 g/mol O x 1 mol O = 15.9994 g O

Molar Mass C10H14O = 150.218 g/mol

Mass % C = 120.170 / 150.218 x 100 = 79.9971 (80%)

Empirical & Molecular Formulas

Empirical formula – formula of a substance written with the smallest whole number subscripts

EF of Acetic Acid = $C_2H_5O_2$

For small molecules, empirical formula is identical to the molecular formula: formula for a single molecule of substance

For Succinic acid, its molecular formula is: $C_4H_6O_4$

Its empirical formula is: $C_2H_3O_2$ (n = 2)

Molecular weight = n x empirical formula weight (n = number of empirical formula units in the molecule)

Practice Problem

Of the following, the only empirical formula is

a. C_2H_4 b. C_5H_{12} c. N_2O_4 d. S_8 e. N_2H_4

Ans: b

Subscript (5) cannot be further divided into whole numbers

Molecular Formula from Elemental Analysis:

A moth repellent, para-dichlorobenzene, has the composition 49.1% C, 2.7% H and 48.2% Cl. Its molecular weight is determined from mass spectrometry. What is its molecular formula?

Assume a sample mass of 100 grams

49.1 g C x 1 mol C /12.0107 g C = 4.0880 mol C

2.7 g H x 1 mol H /1.00794 g H = 2.6787 mol H

48.2 g Cl x 1 mol Cl /35.453 g Cl = 1.3595 mol Cl

Convert Mole values to "Whole" numbers (divide each value by smallest)

4.0880 / 1.3595 = 3.01 (3 mol C)

2.6787 / 1.3595 = 1.97 (2 mol H)

1.3595 / 1.3595 = 1.00 (1 mol Cl)

∴ Empirical Formula is: C_3H_2Cl

Molecular Formula from Elemental Analysis: An Example Calculation (Con't)

Empirical formula = C_3H_2Cl

Compute Empirical Formula Weight (EFW)

EFW= (3 x 12.01) + (2 x 1.01) + (1 x 35.45) = 73.51 g/mol

Molecular weight (M^+ ion from mass spectrum) = 146

n = 146/73.51 = 1.99 = 2

$\therefore$ Molecular Formula = $C_6H_4Cl_2$