

## Calculations in Chemistry

### The Mole

A mole of a substance represents  $6.02 \times 10^{23}$  (Avogadro's number) representative particles of that substance

-it takes  $6.02 \times 10^{23}$  atoms of any element to have a mass equivalent to the atomic mass of the element in grams

For elements:

$$\text{mass (g)} = \# \text{mols} \times \text{atomic mass}$$

for compounds:

$$\text{mass (g)} = \# \text{mols} \times \text{molar mass}$$

$$\# \text{particles} = \# \text{mols} \times 6.02 \times 10^{23}$$

$$\# \text{mols} = \frac{\# \text{particles}}{6.02 \times 10^{23}}$$

or

$$\# \text{mols} = \frac{\text{mass (g)}}{\text{molar mass}}$$

To determine the number of atoms of an element in a compound, multiply the subscript of the element by the number of molecules in compound.

Ex. There are  $2.01 \times 10^{18}$  molecules in 1mg of codeine ( $\text{C}_{18}\text{H}_{21}\text{NO}_3$ ). How many hydrogen atoms in a 1 mg tablet of codeine?

Solution

Multiply  $2.01 \times 10^{18}$  by 21 since there are 21 hydrogens in the formula

$$(2.01 \times 10^{18}) \times 21$$

$$= 4.22 \times 10^{19}$$

### Empirical Formula

Shows the simplest whole number ratio of atoms in a particle of the substance

How to determine it:

1. assume 100% = 100g
2. calculate the number of moles of each of the elements in the given compound
3. divide the number of moles by the smallest number of moles to get the whole number ratio
4. write the empirical formula

### Molecular Formula

Shows the actual number of atoms in a particle of the substance

How to determine it:

1. Find the molar mass of the empirical formula given

2. divide the molar mass of the correct compound by the molar mass of the empirical formula to obtain the whole number multiple of the empirical formula.

Ex. for empirical and molecular formula

You are given a compound made up of 80% carbon, 20% hydrogen, and the molar mass of the compound is 30 g/mol.

Determine:

a) empirical formula

b) molecular formula

Solution

a)	80% C	:	20% H
Assume 100% = 100g			
	$\# \text{mol C} = \frac{80 \text{ g}}{12 \text{ g/mol}}$		$\# \text{mol H} = \frac{20 \text{ g}}{1 \text{ g/mol}}$
	$= 6.67 \text{ mol}$		$= 20 \text{ mol}$
divide by	6.67 mol		6.67 mol
smallest # of	= 1	:	= 3
moles (6.67) to			
get whole # ratio			

$\therefore$  Empirical formula is  $\text{CH}_3$

b)  $M_R \text{CH}_3 = \text{C} + 3\text{H}$   
 $= 12 + (3 \times 1)$   
 $= 15 \text{ g/mol}$

coefficient mult. Factor =  $\frac{M_R \text{ of correct}}{M_R \text{ of E. formula}}$   
 $= \frac{30 \text{ g/mol}}{15 \text{ g/mol}}$   
 $= 2$

$2 (\text{CH}_3)$   
 $= \text{C}_2\text{H}_6$

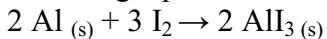
$\therefore$  The molecular formula is  $\text{C}_2\text{H}_6$

### Stoichiometry

Steps:

1. Balanced Equation
2. Grams to moles (use molar mass)
3. Moles to moles (use stoichiometric coefficients from balanced equation)
4. Moles to grams (use molar mass)

Ex. What mass of iodine will react completely with 10.0 g of aluminum according to the following equation:



Solution:

The equation is balanced, so now find the number of moles of Aluminum:

$$\begin{aligned} n &= \frac{10.0 \text{ g}}{27 \text{ g/mol}} \\ &= 0.370 \text{ mol} \end{aligned}$$

$$\text{mol Al} : \text{mol I}_2 = 2 : 3$$

$$\frac{2}{3} = \frac{0.37}{x}$$

$$x = \frac{3 \times 0.37}{2}$$

$$x = 0.555$$

∴ Number of moles of I<sub>2</sub> is 0.555 mol

$$\begin{aligned} \text{mass of I}_2 &= n \times M_R \\ &= 0.555 \times (2 \times 127) \\ &= 140.97 \text{ g} \end{aligned}$$

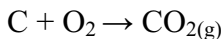
\*A neutralization, or titration, reaction involves reacting an acid with a base to produce a salt and water – use stoichiometry to solve these problems

### Limiting and Excess Reagent Calculations

Limiting reagent: the reactant that is totally consumed, thereby stopping the reaction

Excess reagent: the reactant that is not totally consumed in a reaction

Given 1.0 g of Carbon and 1.0 g of O<sub>2</sub> in the following equation determine which is the limiting reagent, which is in excess, the mass of the excess remaining, and the mass of the CO<sub>2</sub> produced.



Solution

First we must determine the number of moles of each, because grams do not tell us anything:

$$\begin{aligned} n \text{ of C} &= \frac{1.0 \text{ g}}{12.00 \text{ g/mol}} \\ &= 0.083 \text{ mol} \\ &\text{XS} \end{aligned}$$

$$\begin{aligned} n \text{ of O}_2 &= \frac{1.0 \text{ g}}{32 \text{ g/mol}} \\ &= 0.03125 \\ &\text{LR (smaller \# of moles)} \end{aligned}$$

$$\begin{aligned}\text{Moles remaining unreacted} &= 0.083 - 0.03125 \\ &= 0.05175\end{aligned}$$

$$\begin{aligned}\text{Mass of Xs unreacted} &= n \times M_R \\ &= 0.05175 \times 12 \\ &= 0.621\text{g}\end{aligned}$$

To determine the number of moles of CO<sub>2</sub> produced, do a mol to mol ratio with the limiting reagent

$$\begin{aligned}\text{Mol O}_2 &: \text{mol CO}_2 \\ 1 &: 1 \\ \therefore n \text{ CO}_2 &= 0.03125\end{aligned}$$

$$\begin{aligned}\text{Mass CO}_2 &= n \times M_R \\ &= 0.03125 \times 44 \\ &= 1.375 \text{ g}\end{aligned}$$

### **Percentage Yield**

You don't always get 100% of the product that you should theoretically obtain, you get a lower yield. Percent yield is the ratio of the actual yield to the theoretical yield.

Experimental yield: the quantity of product produced in reality (lower due to errors)

Theoretical yield: the quantity of product that should be produced

$$\% \text{ yield} = \frac{\text{Experimental (actual) yield}}{\text{Theoretical yield}} \times 100$$

### **Percent Error**

$$\% \text{ error} = \frac{\text{Theoretical} - \text{Experimental}}{\text{Theoretical}} \times 100$$