Calculations in Chemistry

The Mole

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

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

For elements:
mass (g) = #mols x atomic mass

for compounds:
mass (g)= #mols x molar mass

#particles= #mols x 6.02×10^{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 2.01×10^{18} molecules in 1mg of codeine ($C_{18}H_{21}NO_3$). Howe many hydrogen atoms in a 1 mg tablet of codeine?
<u>Solution</u>
Multiply 2.01×10^{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

<u>Solution</u>

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

:. Empirical formula is CH_3

b) M_R CH_3 = C + 3H
= 12 + (3 x 1)
= 15 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 (CH_3)
=C_2H_6

:. The molecular formula is C_2H_6

<u>Stoichiometry</u>
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:

$2\ Al_{(s)} + 3\ I_2 \rightarrow 2\ AlI_{3\ (s)}$

Solution:

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

$$n = \frac{10.0\ g}{27\ g/mol}$$

$= 0.370$ mol

mol Al : 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_2 is 0.555mol

mass of $I_2 = n \times M_R$

$= 0.555 \times (2 \times 127)$

$= 140.97$ g

*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_2 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_2 produced.

$C + O_2 \rightarrow CO_{2(g)}$

Solution

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

$$n \text{ of } C = \frac{1.0\ g}{12.00\ g/mol}$$

$= 0.083$ mol

XS

$$n \text{ of } O_2 = \frac{1.0\ g}{32\ g/mol}$$

$= 0.03125$

LR (smaller # of moles)

Moles remaining unreacted = 0.083 – 0.03125
= 0.05175

Mass of Xs unreacted = n x M_R
= 0.05175 x 12
= 0.621g

To determine the number of moles of CO_2 produced, do a mol to mol ratio with the limiting reagent

Mol O_2 : mol CO_2
1 : 1
:. n CO_2 = 0.03125

Mass CO_2 = n x M_R
= 0.03125 x 44
= 1.375 g

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

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