Mole Calculations

Chemical Equations and Stoichiometry

<u>Lecture Topics</u>
Atomic weight, Mole, Molecular Mass, Derivation of Formulas, Percent Composition

Chemical Equations and Problems Based on

Miscellaneous Problems, Solution Problems, Review Handout

<u>Demo Mole Quantities</u>

58.5g NaCl(mol/58.5g)(6.02 x 10^{23}/mol) = 6.02 x 10^{23} Na^+Cl^-

21 pre-1982 pennies (after 1982 pennies are mostly zinc with copper coating)
63.5g Cu(mol/ 63.5g)(6.02 x 10^{23}/mol) = 6.02 x 10^{23} Cu

19.0g Al (mol/27.0g)(6.02 x 10^{23}/mol) = 4.24 x 10^{23} Al

<u>Demo of Oxidation Reactions</u>
Flash bulb
$2Mg + O_2 \rightarrow 2MgO$ fast
$2Cn + O_2 \rightarrow 2CnO$ slow

Copper Oxide Penny
$2Cu + O_2 \rightarrow 2CuO$

<u>Intro to Chapter</u>
Stoichiometry is the process of making calculations based on formulas and balanced equations

Since Modern Chemistry involves:
- Symbolic representation of models
- Mathematics
- Quantitative measurements

You are going to be using lots of symbols and equations and doing lots of calculations

The fundamental Question –
How do you go from combining ratio of atoms (like H_2O) to something you can measure in lab?
OR How do you go between number of atoms and mass of that collection of atoms?

Mole abbreviation is **mol**
Molecular and formula weight

Suppose we want to make CO_2, we burn coal because mainly carbon
$C + O_2 \rightarrow CO_2$
Carbon + Oxygen = Carbon Dioxide

Ratio of atoms of oxygen to carbon is 2:1
Do this in lab, will not work with single atoms and molecules but a large number that we determine by finding mass

The special number we use, **Avogadro's number** (**6.022×10^{23}**) is called a **mole** and is the amount of substance that contains 6.022×10^{23} units of that substance

Avogadro's number is based on Carbon standard ^{12}C so that 12.0000 g of the 12C isotope contains 6.022×10^{23} carbon atoms

If this seems confusing think of dozen (it is a word that means 12)
Ex: get me 2 dozen glaze doughnuts 2 dozen = 2 (12) = 24

Ex: give me 2 moles of copper atoms 2 mol = 2 (6.022×10^{23}) = 1.204×10^{23} Cu atoms

Molar Mass (MM) or Molecular Weight (MW) or Formula Weight (FW) all same thing
Atomic mass (or older term atomic weight) of element contains 1 mol of atoms
Ex: 6.02×10^{23} Cu atoms have a mass of 63.5g

12.0g C + 32.0g $O_2 \rightarrow$ 44.0g CO_2 (12.0 + 16.0 + 16.0 = 44.0g)
1 mol 1 mol 1 mol

Number $\rightarrow$ molecular weight or atomic weight $\rightarrow$ mass

Made of ions or atoms = formula weight
Formula weight is the sum of the atomic weight in the formula

Made of molecules = Molecular (or Molar) Mass
Molecular weight is the sum of atomic weights in molecule

NaCl 1 mol (Na) + 1 mol (Cl) = 23.0 g/mol + 35.5 g/mol = 58.5 g/mol

H_2O 2 mol (H) + 1 mol (O) = 2(1.0 g/mol) + 1(16.0 g/mol) = 18.0 g/mol

How many moles, atoms in 3.05g copper penny?
? mol Cu = 3.05g Cu (1 mol Cu/ 63.5g Cu) = 0.0480 mol Cu = 4.80×10^{-2} mol

? atoms Cu = 4.80 x 10^{-2} mol Cu (6.022 x 10^{23} atoms Cu/ mol Cu) = 2.89 x 10^{22} atoms Cu

To realize how big number above is think of person 100 years old who has had
?seconds in life = 100yr (365day/yr) (24hr/day) (60min/hr) (60s/hr)
= 3.15 x 10^9 seconds in life

Find the molecular weight of CH_4 (methane)

Atomic weight: C = 12.01 g/mol
H = 1.01 g/mol
1(C) + 4(H)
1 mol CH_4 = (1mol)(12.01 g/mol) + (4 mol)(1.01 g/mol) = 16.05 g

Find formula weight $MgCl_2$ (magnesium chloride)

?g = 1 mol $MgCl_2$ = (1 mol)(24.3g/mol) + (2 mol)(35.5g/mol) = 95.3g
95.3 g/mol

1 mole means 6.022 x 10^{23} units of specified entity ($MgCl_2$, CH_4, C, etc.)

Terms used: Molar mass ~ Molecular weight ~ Formula weight
This means the terms are interchangeable:
For 1 mole of CO_2 = 44.0 g/mol
For 1 average molecule of CO_2 = 44.0 amu

Derivation of Formulas and Percent Composition

percent composition ⇔ atomic masses ⇔ empirical formula
(from Periodic Table)

empirical formula ⇔ molar mass ⇔ molecular formula
(given based on Expt.)

Given % find Empirical Formula and
then given Molar Mass find Molecular Formula

consider Glucose which is the sugar in I.V. fluids

Given: 40.0% C
6.73% H
53.3% O
and Molecular Weight= 180.2 g/mol

1) Find Empirical Formula
Steps: 1. Assume 100g sample 40.0g C 6.73g H 53.3g O
2. Convert g to mol
3. Find ratio

? mol C = (40.0g)(1 mol/ 12.0g) = 3.33 ~ 1
? mol H = (6.73g)(1 mol/ 1.01g) = 6.73 ~2
? mol O = (53.3g)(1mol/ 16.0g) = 3.33 ~ 1

H/O = 6.73/3.33= 2/1
C/O = 3.33/3.33 = 1/1
$\mathbf{C_1H_2O_1}$

2) Find Molecular Formula
Empirical weight = 30g

(EW)(n) = (MW) Empirical Weight times something equal Molecular Weight
(30g/mol)(6) = (180.2 g/mol)

so need 6 $C_1H_2O_1$ groups together to make $\mathbf{C_6H_{12}O_6}$

<u>Calculation of Percent Composition</u>

To calculate % composition from formula
Steps: 1. Assume 1 mole
2. Convert to grams
3. Calculate %

Example:
SnF2 (stannous fluoride)
tin (II) fluorine
This is a historically active ingredient

Sn 1 mol (119g/mol) = 119g
F 2 mol (19 g/mol) = 38g

1 mol weight 119 + 19 + 19 = 157.0 g/mol (Molecular Weight)

% Sn by weight (119.0/157.0) x 100% = 75.8% tin

% F by weight (38.0/ 157.0) x 100% = 24.2% fluorine

75.8% + 24.2% = 100%

Chemical Equations and Problems

Symbolic representation of chemical reactions
Rearrangements of atoms is the central idea to chemistry and science
Examples:
Transformation of matter
Refining a metal
Making nylon stockings
Synthesizing a new medicine

Flash bulb	magnesium + oxygen			-->	magnesium oxide
		(reactants)		*(yields)*	*(products)*
	Mg	+	O_2	-->	MgO
	2Mg	+	O_2	-->	2MgO
	aluminum + oxygen			-->	aluminum oxide
	Al	+	O_2	-->	Al_2O_3
	4Al	+	$3O_2$	-->	$2Al_2O_3$

Balance Chemical Equation

1. Use given molecules, do NOT change subscripts, subscripts tell us how many atoms in molecule based on experimental observation
2. DO change prefix numbers
3. Save simpler elements until last
4. Convert to whole number coefficients
5. Check your answer

CH_4	+	O_2	-->	CO_2	+	H_2O
CH_4	+	O_2	-->	CO_2	+	$2H_2O$
$1CH_4$	+	O_2	-->	$1CO_2$	+	$2H_2O$
$1CH_4$	+	$2O_2$	-->	$1CO_2$	+	$2H_2O$

Note: If the compound only appears once on each side then start with that molecule

Reactants	Products
1C	1C
4H	4H
4O	4O

Mass is conserved
Heat is given off but energy is conserved
Potential to Kinetic

Stoichiometry problems are based on chemical equations
reactants --> products

Types of questions asked:
How much products formed?
How much reactants used up?
Could be asked for in the units moles, atoms, grams

Example:
NH_3 + F_2 ---> N_2F_4 + HF

Balance reaction
$2NH_3$ + $5F_2$ ---> N_2F_4 + 6HF

Problem Type: One quantity given

Given excess NH_3 114g F_2 How much N_2F_4?

mass A --> (MW)--> mol A -->(balance equation)-->mol B -->(MW)-->mass B =114g F_2

? mol N_2F_4 = (114g F_2)(1 mol F_2/ 38g F_2)(1 mol N_2F_4/ 5 mol F_2)(104g N_2F_4/ mol N_2F_4)
? g N_2F_4 = 62.4g N_2F_4

Rules: 1. Indicates mass of substance given
2. Convert mass to moles (molecular weight)
3. Enter conversion factor from balanced equation
4. Convert moles to mass of substance sought (molecular weight)
5. Carry out math

Miscellaneous Problems
Example: How much of one type of element in a compound?

How many **grams of silver** (Ag) in 300g of silver(I) sulfide ore called argentite (Ag_2S)

Ag_2S = (2 mol)(108 g/mol) + (1 mol)(32.1 g/ mol) = 248.1 g
and in above 248.1g or ore there are 2 mol Ag = 2(108 g/mol) = 216 g
so (216g Ag/ 248.1g Ag_2S)
and then
?g Ag = 300g Ag_2S (216g Ag/ 248.1g Ag_2S)

= **261g Ag**

OR

?g Ag = 300g Ag_2S(1 mol Ag_2S/ 248.1 Ag_2S)(2 mol Ag/1 mol Ag_2S)(108g Ag/mol Ag)
= 261g Ag

mass → moles → ratio moles→ mass

Percentage Yield

Theoretical yield is the amount of product if reaction goes to completion (100%)

Actual Yield is the amount of product actually obtained

Percentage Yield = (actual/theoretical) x 100%

Expect 400g of CaCO3
Get 300g
Percentage Yield = 300/400 x 100% = 75%

Problem type: More than one quantity given. Find the Limiting Reactant

Steps:
1. Calculate moles of each of reactants
2. Divide the actual moles by needed moles in equation
3. Smaller number is the limiting reactant, use this value for calculation

$2NH_3 + 5F_2 \rightarrow N_2F_4 + 6HF$
Given: 152g F_2 and 55g NH_3 --> ?g HF

F_2 (152g)(1 mol/38g) = 4.00 mol
(actual/ needed) = 4/5 = 0.80 (F_2 is the Limiting Reactant)

NH_3 (55.0g)(1 mol/17g) = 3.24 mol
(actual/needed) = 3.24/2 = 1.62 (excess)

Work the rest of the problems in this same manner

?g N_2F_4 = (152g F_2)(1 mol F_2/ 38g F_2)(6 mol HF/ 5 mol F_2)(20g HF/ mol HF)=96g HF
4.8 mol HF

Needed Ratio 5 F_2/2 NH_3 = 2.5
Actual Ratio: 4 F_2/ 3.24 NH_3 = 1.24
So not enough F_2
F_2 is the Limiting Reactant

Stoichiometry of Solutions
Concentration is the amount of substance dissolved in volume of solution
Ex: Coffee: 1 teaspoon/cup
2 teaspoon/cup
3 teaspoon/cup

Coffee Crystals – Solute
Water – Solvent
Coffee – Solution

Use Molarity (M) = moles of solute/ L of solution

Ex1:
Penny ~ 3g
Cu .1mol/L
Mol Cu = 63.5g
2 pennys/L
Not dissolved so therefore there is no solution

Ex2:
NaCl 58.5g/mol
5.85g dissolved into a total solution volume of 1.00 L
5.85g/ 1 Liter = 0.100 mol/L= 0.10M NaCl(aq) that is Na^+ and Cl^- ions
NaCl dissolve into ions (but other solutions like sugar may be made of dissolved molecules)

Moles and volume in solution use molarity
concentration (mol/L) so mol ← (conc) → volume

Note: Concentration is the conversion factor between moles and volume
moles = (**concentration)(volume)**
mol = (L) (mol/L)

1000ml = 1L
250ml of 0.20M NaCl
(0.20 mol/L NaCl)(250ml)(1 L/ 1000ml) = 0.050 mol NaCl
(**concentration)(volume) = moles**

Different than previous problems because it can be asked what volumes should be combined

0.1M NaCl Na^+ Cl^- =.1M
0.1M $MgCl_2$ $Mg2^+$ $2Cl^-$ = .2M

Preparation of Solution

How many grams of NaOH to prepare a 0.75M solution of 250ml (.250L)?

?g NaOH = (0.75 mol NaOH/L)(250ml)(1L/ 100ml)(40.0g NaOH/ mol NaOH)
= 7.50g NaOH

Suggestions: Convert milliliters to liters
Always include units

Dilution of Solution

$M_1V_1 = M_2V_2$

What volume of 5.00M HCl to dilute to 100ml of 1.00M HCl (aq)?

$M_1 = 5.0$ $V_1 = ?$ ml
$M_2 = 1.0$ $V_2 = 100$ml

Solve equation find $V_1 = 20$ ml

More Miscellaneous Practice Problems

Find Molecular weight NaOH Given: Periodic Table
To Do: 23.0 + 16.0 + 1.0 = 40.0 g/mol

Convert 10.0g NaOH to mol of NaOH
? mol = (10.0g NaOH)(mol NaOH/ 40.0g NaOH) = 0.250 mol

Convert 2.0mol of NaOH to g
? g = (2.0 mol NaOH)(40.0g NaOH/ mol NaOH) = 80g NaOH

Convert 0.250mol NaOH to number of sodium ions
? ions of Na^+ = (0.250 mol)(6.02×10^{23}/mol) = 1.50×10^{23} Na^+

Convert 1.2×10^{24} sodium ions to moles
? mol = (1.2×10^{24} ions)(mol/6.02×10^{23}) = 2 mol Na^+

Find concentration of 20.1g of NaOH in 300 mL volume of solution

?M = ? mol/L = [20.1g (mol/40.0g)] / [300mL (1 L / 1000mL)]
= 0.503mol/ 0.300L
= 1.68 M NaOH(aq)

DEMO

Put methanol in a plastic bottle
Allow vapor to spread and introduce flame at top
Spread to bottom of the jar
Burns down as air rushes in

CH_3OH methanol combustion may be written as:

$CH_4O + 3/2O_2 \rightarrow CO_2 + 2H_2O$ + energy (light and heat)

$2CH_4 + 3O_2 \rightarrow 2CO_2 + 4H_2O$ + energy

this is Exothermic reaction because it gives off heat

Summary of Stoichiometry Conversions

To Find	Given	Need to	Example
Molar Mass*	periodic table	sum atomic masses	find molecular weight (formula mass) of NaOH ? g/mol = Na + O + H = 23.0 + 16.0 + 1.0 = 40.0 g/mol
mole	mass	(mass) (1/W)	find the moles of 10.0 grams of NaOH ? mol = (10.0g NaOH)(1mol/40.0g) = 0.250 mol NaOH
mass	mole	(mol) (W)	find the mass of 2.00 moles of NaOH ?g = (2.00molNaOH)(40.0 g/mol) = 80.0 g NaOH
mole	number	number (1/N)	find the moles in $12x10^{23}$ molecules of water ? mol = $(12x10^{23})$ $(mol/6.02x10^{23})$ = 2.0 mol
number	mole	(mol) (N)	find the number of OH^- in 0.25mol of $Ca(OH)_2$? OH^- = (2OH-)(0.25mol)($6.02x10^{23}$/mol) = $3.0x10^{23}$ OH^-
mole	volume	(V) (conc)	find moles of Cl^- in a 250mL of 0.500M HCl(aq) ? mol Cl- = (0.250L) (0.50 mol/L) = 0.125 mol Cl^-
volume	mole	(mol)(1/conc)	find volume of 0.50M HCl(aq) to have 2.0 mol Cl- ? L = (2.0mol)(L / 0.50mol) = 4.0 L

Symbols Used

conc concentration is commonly expressed as molarity M (mol/L)

N Avogadro's number $6.02x10^{23}$ /mol

V volume of solution

W molecular weight or molar mass or formula weight *Note we will tend to use any of the terms molar mass or molar weight or molecular weight for mass of a mole of compound. To be more precise if compound does not exist as molecules we can use the term formula mass or formula weight. Most of the time chemists just say molecular weight for the mass of a mole of compound regardless of whether it exists as molecules or not.

To convert between

moles and mass use molecular weight (g/mol)	mol ← (W) → mass
moles and number use Avogadro's number 6.02×10^{23} mol^{-1}	mol ← (N) → number
moles and volume in solution use molarity concentration (mol/L)	mol ← (conc) → volume