

Mole Calculations

Chemical Equations and Stoichiometry

Lecture Topics

Atomic weight, Mole, Molecular Mass, Derivation of Formulas, Percent Composition

Chemical Equations and Problems Based on

Miscellaneous Problems, Solution Problems, Review Handout

Demo Mole Quantities

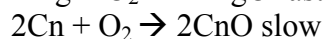
$$58.5\text{g NaCl}(\text{mol}/58.5\text{g})(6.02 \times 10^{23}/\text{mol}) = 6.02 \times 10^{23} \text{ Na}^+\text{Cl}^-$$

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

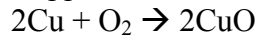
$$19.0\text{g Al}(\text{mol}/27.0\text{g})(6.02 \times 10^{23}/\text{mol}) = 4.24 \times 10^{23} \text{ Al}$$

Demo of Oxidation Reactions

Flash bulb



Copper Oxide Penny



Intro to Chapter

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

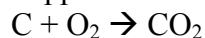
The fundamental Question –

How do you go from combining ratio of atoms (like H₂O) 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 CO₂, we burn coal because mainly carbon



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 ¹²C 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)

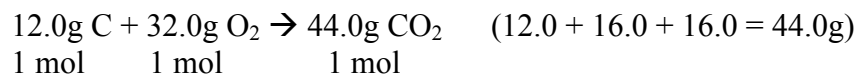
Ex: get me 2 dozen glaze doughnuts 2 dozen = 2 (12) = 24

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



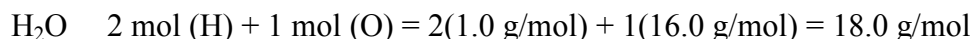
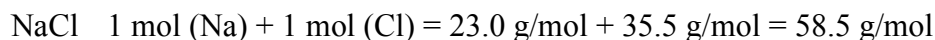
Number → molecular weight or atomic weight → mass

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



How many moles, atoms in 3.05g copper penny?

$$? \text{ mol Cu} = 3.05\text{g Cu} \left(\frac{1 \text{ mol Cu}}{63.5 \text{ g Cu}} \right) = 0.0480 \text{ mol Cu} = 4.80 \times 10^{-2} \text{ mol}$$

$$? \text{ atoms Cu} = 4.80 \times 10^{-2} \text{ mol Cu} (6.022 \times 10^{23} \text{ atoms Cu/ mol Cu}) = 2.89 \times 10^{22} \text{ atoms Cu}$$

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)
= 3.15×10^9 seconds in life

Find the molecular weight of CH₄ (methane)

Atomic weight: C = 12.01 g/mol

H = 1.01 g/mol

1(C) + 4(H)

$$1 \text{ mol CH}_4 = (1 \text{ mol})(12.01 \text{ g/mol}) + (4 \text{ mol})(1.01 \text{ g/mol}) = 16.05 \text{ g}$$

Find formula weight MgCl₂ (magnesium chloride)

$$?g = 1 \text{ mol MgCl}_2 = (1 \text{ mol})(24.3 \text{ g/mol}) + (2 \text{ mol})(35.5 \text{ g/mol}) = 95.3 \text{ g}$$

95.3 g/mol

1 mole means 6.022×10^{23} units of specified entity (MgCl₂, CH₄, C, etc.)

Terms used: Molar mass ~ Molecular weight ~ Formula weight

This means the terms are interchangeable:

For 1 mole of CO₂ = 44.0 g/mol

For 1 average molecule of CO₂ = 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

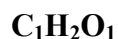
$$? \text{ mol C} = (40.0\text{g})(1 \text{ mol} / 12.0\text{g}) = 3.33 \sim 1$$

$$? \text{ mol H} = (6.73\text{g})(1 \text{ mol} / 1.01\text{g}) = 6.73 \sim 2$$

$$? \text{ mol O} = (53.3\text{g})(1\text{mol} / 16.0\text{g}) = 3.33 \sim 1$$

$$\text{H/O} = 6.73/3.33 = 2/1$$

$$\text{C/O} = 3.33/3.33 = 1/1$$



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 $C_6H_{12}O_6$

Calculation of Percent Composition

To calculate % composition from formula

Steps: 1. Assume 1 mole
2. Convert to grams
3. Calculate %

Example:

SnF_2 (stannous fluoride)

tin (II) fluoride

This is a historically active ingredient

$$\text{Sn} \quad 1 \text{ mol} (119\text{g/mol}) = 119\text{g}$$

$$\text{F} \quad 2 \text{ mol} (19 \text{ g/mol}) = 38\text{g}$$

$$1 \text{ mol weight } 119 + 19 + 19 = 157.0 \text{ g/mol (Molecular Weight)}$$

$$\% \text{ Sn by weight } (119.0/157.0) \times 100\% = 75.8\% \text{ tin}$$

% F by weight $(38.0 / 157.0) \times 100\% = 24.2\%$ 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

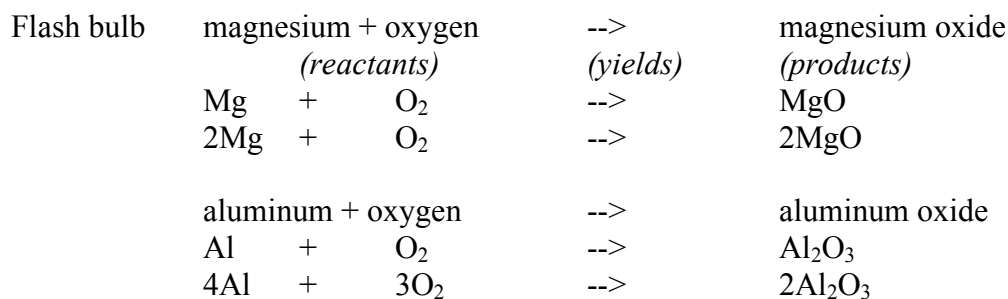
Examples:

Transformation of matter

Refining a metal

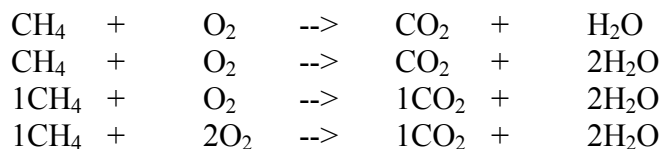
Making nylon stockings

Synthesizing a new medicine



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



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

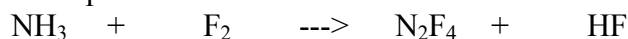


Mass is conserved
Heat is given off but energy is conserved
Potential to Kinetic

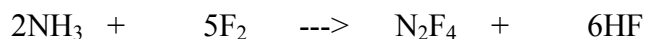
Stoichiometry problems are based on chemical equations
reactants --> products

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

Example:



Balance reaction



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)

$\text{Ag}_2\text{S} = (2 \text{ mol})(108 \text{ g/mol}) + (1 \text{ mol})(32.1 \text{ g/mol}) = 248.1 \text{ g}$
and in above 248.1g of 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)

$$= 261\text{g Ag}$$

OR

$$\begin{aligned} ?\text{g Ag} &= 300\text{g Ag}_2\text{S} \left(\frac{1 \text{ mol Ag}_2\text{S}}{248.1 \text{ Ag}_2\text{S}} \right) \left(\frac{2 \text{ mol Ag}}{1 \text{ mol Ag}_2\text{S}} \right) (108\text{g Ag/mol Ag}) \\ &= 261\text{g Ag} \end{aligned}$$

mass \rightarrow moles \rightarrow ratio moles \rightarrow 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

$$\text{Percentage Yield} = (\text{actual/theoretical}) \times 100\%$$

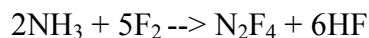
Expect 400g of CaCO₃

Get 300g

$$\text{Percentage Yield} = 300/400 \times 100\% = 75\%$$

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



Given: 152g F₂ and 55g NH₃ \rightarrow ?g HF

$$\begin{aligned} \text{F}_2 (152\text{g}) \left(\frac{1 \text{ mol}}{38\text{g}} \right) &= 4.00 \text{ mol} \\ (\text{actual/ needed}) &= 4/5 = 0.80 \text{ (F}_2 \text{ is the Limiting Reactant)} \end{aligned}$$

$$\begin{aligned} \text{NH}_3 (55.0\text{g}) \left(\frac{1 \text{ mol}}{17\text{g}} \right) &= 3.24 \text{ mol} \\ (\text{actual/needed}) &= 3.24/2 = 1.62 \text{ (excess)} \end{aligned}$$

Work the rest of the problems in this same manner

$$\begin{aligned} ?\text{g N}_2\text{F}_4 &= (152\text{g F}_2) \left(\frac{1 \text{ mol F}_2}{38\text{g F}_2} \right) \left(\frac{6 \text{ mol HF}}{5 \text{ mol F}_2} \right) (20\text{g HF/mol HF}) = 96\text{g HF} \\ &4.8 \text{ mol HF} \end{aligned}$$

$$\text{Needed Ratio } 5 \text{ F}_2 / 2 \text{ NH}_3 = 2.5$$

$$\text{Actual Ratio: } 4 \text{ F}_2 / 3.24 \text{ NH}_3 = 1.24$$

So not enough F₂

F₂ 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 MgCl₂ Mg²⁺ 2Cl⁻ = .2M

Preparation of Solution

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

$$\begin{aligned} ?g \text{ NaOH} &= (0.75 \text{ mol NaOH/L})(250\text{ml})(1\text{L} / 100\text{ml})(40.0\text{g NaOH} / \text{mol NaOH}) \\ &= 7.50\text{g NaOH} \end{aligned}$$

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)?

$$\begin{aligned} M_1 &= 5.0 & V_1 &= ? \text{ ml} \\ M_2 &= 1.0 & V_2 &= 100\text{ml} \end{aligned}$$

Solve equation find $V_1 = 20 \text{ ml}$

More Miscellaneous Practice Problems

Find Molecular weight NaOH Given: Periodic Table

$$\text{To Do: } 23.0 + 16.0 + 1.0 = 40.0 \text{ g/mol}$$

Convert 10.0g NaOH to mol of NaOH

$$? \text{ mol} = (10.0\text{g NaOH})(\text{mol NaOH} / 40.0\text{g NaOH}) = 0.250 \text{ mol}$$

Convert 2.0mol of NaOH to g

$$? \text{ g} = (2.0 \text{ mol NaOH})(40.0\text{g NaOH} / \text{mol NaOH}) = 80\text{g NaOH}$$

Convert 0.250mol NaOH to number of sodium ions

$$? \text{ ions of Na}^+ = (0.250 \text{ mol})(6.02 \times 10^{23} / \text{mol}) = 1.50 \times 10^{23} \text{ Na}^+$$

Convert 1.2×10^{24} sodium ions to moles

$$? \text{ mol} = (1.2 \times 10^{24} \text{ ions})(\text{mol} / 6.02 \times 10^{23}) = 2 \text{ mol Na}^+$$

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

$$\begin{aligned} ?M &= ? \text{ mol/L} = [20.1 \text{ g} (\text{mol} / 40.0\text{g})] / [300\text{mL} (1 \text{ L} / 1000\text{mL})] \\ &= 0.503\text{mol} / 0.300\text{L} \\ &= 1.68 \text{ M NaOH(aq)} \end{aligned}$$

DEMO

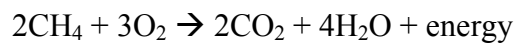
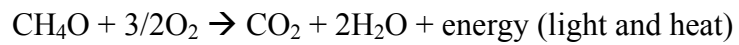
Put methanol in a plastic bottle

Allow vapor to spread and introduce flame at top

Spread to bottom of the jar

Burns down as air rushes in

CH₃OH methanol combustion may be written as:



this is Exothermic reaction because it gives off heat

Summary of Stoichiometry Conversions

<u>To Find</u>	<u>Given</u>	<u>Need to</u>	<u>Example</u>
Molar Mass*	periodic table	sum atomic masses	find molecular weight (formula mass) of NaOH $? \text{ g/mol} = \text{Na} + \text{O} + \text{H}$ $= 23.0 + 16.0 + 1.0$ $= 40.0 \text{ g/mol}$
mole	mass	(mass) (1/W)	find the moles of 10.0 grams of NaOH $? \text{ mol} = (10.0\text{g NaOH})(1\text{mol}/40.0\text{g})$ $= 0.250 \text{ mol NaOH}$
mass	mole	(mol) (W)	find the mass of 2.00 moles of NaOH $? \text{ g} = (2.00\text{molNaOH})(40.0 \text{ g/mol})$ $= 80.0 \text{ g NaOH}$
mole	number	number (1/N)	find the moles in 12×10^{23} molecules of water $? \text{ mol} = (12 \times 10^{23}) (\text{mol}/6.02 \times 10^{23})$ $= 2.0 \text{ mol}$
number	mole	(mol) (N)	find the number of OH ⁻ in 0.25mol of Ca(OH) ₂ $? \text{ OH}^- = (2\text{OH}^-)(0.25\text{mol})(6.02 \times 10^{23}/\text{mol})$ $= 3.0 \times 10^{23} \text{ OH}^-$
mole	volume	(V) (conc)	find moles of Cl ⁻ in a 250mL of 0.500M HCl(aq) $? \text{ mol Cl}^- = (0.250\text{L})(0.50 \text{ mol/L})$ $= 0.125 \text{ mol Cl}^-$
volume	mole	(mol)(1/conc)	find volume of 0.50M HCl(aq) to have 2.0 mol Cl ⁻ $? \text{ L} = (2.0\text{mol})(\text{L} / 0.50\text{mol})$ $= 4.0 \text{ L}$

Symbols Used

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

N Avogadro's number $6.02 \times 10^{23} / \text{mol}$

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)

moles and number use Avogadro's number $6.02 \times 10^{23} \text{ mol}^{-1}$

moles and volume in solution use molarity concentration (mol/L)

mol \leftarrow (W) \rightarrow mass

mol \leftarrow (N) \rightarrow number

mol \leftarrow (conc) \rightarrow volume