

Chapter 3

Calculation with Chemical Formulas and Equations

Practical Applications of Chemistry

- Determining chemical formula of a substance
- Predicting the amount of substances consumed during a reaction
- Predicting the amount of substances produced during a reaction

Example:

Polymer chemist is preparing a new plastic and want to know how much material will a particular reaction yield?

Chemical engineer and is working on a rocket engine thrust. He needs to calculate the amount of exhaust certain gas fuel will produce.

An environmental chemist examining the quality of air pollutants. She is examining what a sample of coal will release into the air when burned.

I) Molecular Weight, Moles and Molar Mass

A) Molecular weight/Formula weight

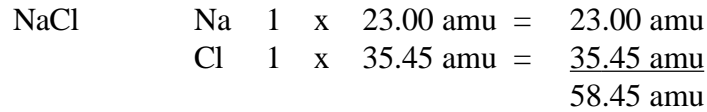
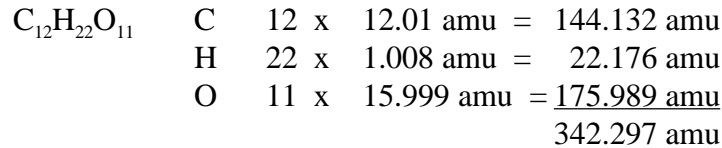
The term **molecular weight** is used with covalent molecules, whereas **formula weight** is used with ionic compounds. Both terms have the same units and are calculated in the same way.

- Sum of the atomic weights of all atoms in the compound
- units of amu (atomic mass units)
- abbreviated
MW - molecular weight
FW - formula weight

Example

Calculate the MW or FW for the following substances

H ₂ O	H	2	x	1.008 amu	=	2.016 amu
	O	1	x	15.99 amu	=	<u>15.999 amu</u>
						18.015 amu



B) Moles

Mole is a chemist counting unit

- used to count atoms, molecules, or compounds by weighting
- abbreviation: mol
- 1 mol objects = 6.02×10^{23} objects

 Avogadro's Number

similar to 1 doz. eggs = 12 eggs

1 mole C atoms = 6.02×10^{23} C atoms

1 mole H_2O molecules = 6.02×10^{23} H_2O molecules

1 mol NaCl = 6.02×10^{23} NaCl formula units

Calculation:

If 1 mole $CaCl_2$ = 6.02×10^{23} $CaCl_2$ formula units, How many Cl^- ions are in 1 mole of $CaCl_2$?

1 mole of $CaCl_2$ consists of 1 mole Ca^{2+} and 2 mole Cl^- . If 1 mole of Cl^- is 6.02×10^{23} Cl^- ions, then 1 mole of $CaCl_2$ contains $(2 \times 6.02 \times 10^{23})$ Cl^- ions or 1.20×10^{24} Cl^- ions.

C) Molar Mass

What is the mass of 1 mole of a substance?

Molar mass

- mass of 1 mole of a substance
- numerically equal to the MW or FW
- units of g/mol
- my abbreviation for molar mass is M_m

example:

substance	MW or FW	molar mass
Fe	55.847 amu	55.847 g/mol
H ₂ O	18.015 amu	18.015 g/mol
C ₁₂ H ₂₂ O ₁₁	342.297 amu	342.297 g/mol
NaCl	58.45 amu	58.45 g/mol

Calculations:

Molar mass is useful in converting between units of grams and moles

example:

How many grams of Ag are in 0.750 mol Ag?

Ag: $M_m = 107.9 \text{ g/mol}$

$$0.750 \text{ mol} \left(\frac{107.9 \text{ g}}{1 \text{ mol}} \right) = 80.9 \text{ g Ag}$$

How many mole of NaCl are in 118.0 g NaCl?

NaCl: $M_m = 58.45 \text{ g/mol}$

$$118.0 \text{ g} \left(\frac{1 \text{ mol}}{58.45 \text{ g}} \right) = 2.019 \text{ mol NaCl}$$

How many molecules of H₂O are in 22.0 g H₂O?

H₂O: $M_m = 18.015 \text{ g/mol}$

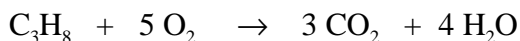
$$22.0 \text{ g H}_2\text{O} \left(\frac{1 \text{ mol H}_2\text{O}}{18.0 \text{ g H}_2\text{O}} \right) \left(\frac{6.02 \times 10^{23} \text{ molecules}}{1 \text{ mol H}_2\text{O}} \right) = 7.36 \times 10^{23} \text{ H}_2\text{O molecules}$$

II) Stoichiometry

A) Molar interpretation of chemical equation

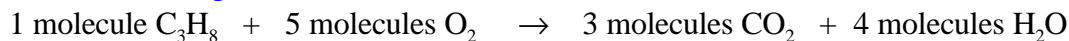
The coefficients within a chemical reaction indicate the number of molecules, formula units or moles of substance in needed or produced.

for example, observe the coefficients in the following combustion reaction.

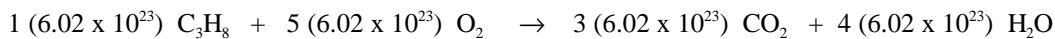


What do the coefficients represent in a chemical reaction?

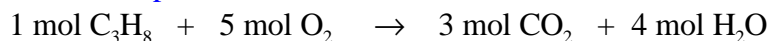
Molecular interpretation:



If each of the coefficients are multiplied by avogadro's number, the coefficients now represent the number of moles of each substance



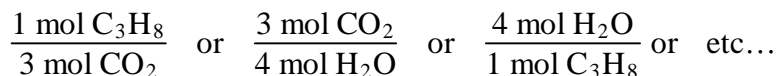
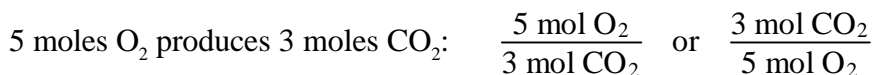
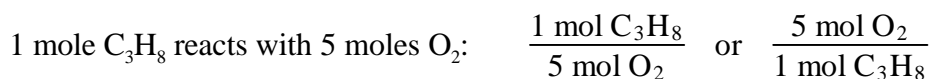
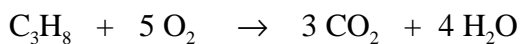
Molar interpretation:



B) Amounts of substances in a chemical reaction

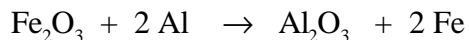
Mole ratios of reactants and products can be written from a balance chemical reaction. These mole ratios are conversion factors, which converts from moles of one substance to moles of another substance.

Using the following chemical reaction, several conversion factors (mole ratios) can be written.



example:

Thermite is a mixture of iron(III) oxide and aluminum powders that were once used to weld railroad tracks. It undergoes a spectacular reaction to yield solid aluminum oxide and molten iron.



How many mole Al_2O_3 are produced from 12.0 mol Al?

$$12.0 \text{ mol Al} \left(\frac{1 \text{ mol Al}_2\text{O}_3}{2 \text{ mol Al}} \right) = 6.00 \text{ mol Al}_2\text{O}_3$$

How many grams of iron form when 135 g Al react?

$$135 \text{ g Al} \left(\frac{1 \text{ mol Al}}{27.0 \text{ g Al}} \right) \left(\frac{2 \text{ mol Fe}}{2 \text{ mol Al}} \right) \left(\frac{55.8 \text{ g Fe}}{1 \text{ mol Fe}} \right) = 279 \text{ g Fe}$$

How many atoms of Al react for every 1.00 g Al_2O_3 that forms?

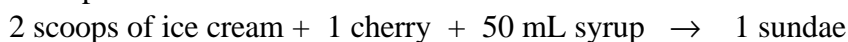
$$1.00 \text{ g Al}_2\text{O}_3 \left(\frac{1 \text{ mol Al}_2\text{O}_3}{102 \text{ g Al}_2\text{O}_3} \right) \left(\frac{2 \text{ mol Al}}{1 \text{ mol Al}_2\text{O}_3} \right) \left(\frac{6.02 \times 10^{23} \text{ Al atoms}}{1 \text{ mol Al}} \right) = 1.18 \times 10^{22} \text{ Al atoms}$$

C) Limiting reactants (limiting reagents)

- 1) The reactant which is used up entirely during the reaction is the **limiting reagent**
- 2) The reactant which is left over after the limiting reagent is used up is the **excess reagent**

To determine which reagent or reactant is limiting, calculate the amount of product that can be formed with each reactant. The reactant that produces the least amount of product is the limiting reagent. The other reactants are considered the excess reagents.

Example:



How many sundaes can be if 50 scoops of ice cream, 30 cherries and 1 L of syrup are available?

$$50 \text{ scoops} \left(\frac{1 \text{ sundae}}{2 \text{ scoops}} \right) = 25 \text{ sundaes}$$

$$30 \text{ cherries} \left(\frac{1 \text{ sundae}}{1 \text{ cherry}} \right) = 30 \text{ sundaes}$$

$$1000 \text{ mL syrup} \left(\frac{1 \text{ sundae}}{50 \text{ mL syrup}} \right) = 20 \text{ sundaes}$$

The syrup will run out first before the ice cream or cherries, so it is the limiting reagent, while the ice cream and cherries are the reagents in excess.

A limiting reagent problem in chemistry usually involves determining the amount of a product that can be formed given the various amounts of reactants mixed together in the reaction.

For example:

- a) Calculate the mass of iodic acid (HIO_3) that forms when 735 g iodine trichloride reacts with 97.7 g water.



- 1) Calculate the number of moles of HIO_3 produced with each one of the reactants.

$$735 \text{ g ICl}_3 \left(\frac{1 \text{ mol ICl}_3}{233.4 \text{ g ICl}_3} \right) \left(\frac{1 \text{ mol HIO}_3}{2 \text{ mol ICl}_3} \right) = 1.57 \text{ mol HIO}_3$$

$$97.7 \text{ g H}_2\text{O} \left(\frac{1 \text{ mol H}_2\text{O}}{18.0 \text{ g H}_2\text{O}} \right) \left(\frac{1 \text{ mol HIO}_3}{3 \text{ mol H}_2\text{O}} \right) = 1.81 \text{ mol HIO}_3$$

- 2) Because ICl_3 produces the lesser amount of product, it is the limiting reagent. Use 1.57 mol HIO_3 to calculate the mass.

$$1.57 \text{ mol HIO}_3 \left(\frac{175.9 \text{ g HIO}_3}{1 \text{ mol HIO}_3} \right) = 276 \text{ g HIO}_3$$

- b) Now calculate the mass of the excess reagent remaining after the reaction in question 1 is completed.

- 1) Using the amount of product produced by the limiting reagent, back calculate the mass of the excess reagent used in the reaction.

$$1.57 \text{ mol HIO}_3 \left(\frac{3 \text{ mol H}_2\text{O}}{1 \text{ mol HIO}_3} \right) \left(\frac{18.0 \text{ g H}_2\text{O}}{1 \text{ mol H}_2\text{O}} \right) = 84.8 \text{ g H}_2\text{O used}$$

- 2) To find the amount of excess reagent remaining, subtract the amount used in the reaction from the given amount at the beginning of the reaction.

$$\begin{aligned} \text{starting mass} - \text{mass used} &= \text{mass remaining} \\ 97.7 \text{ g} - 84.8 \text{ g} &= 12.9 \text{ g H}_2\text{O remaining} \end{aligned}$$

3. How many grams of solid aluminum sulfide can be prepared by the reaction of 10.0 g aluminum and 15.0 g sulfur?



$$10.0 \text{ g Al} \left(\frac{1 \text{ mol Al}}{27.0 \text{ g Al}} \right) \left(\frac{1 \text{ mol Al}_2\text{S}_3}{2 \text{ mol Al}} \right) = 0.185 \text{ mol Al}_2\text{S}_3$$

$$15.0 \text{ g S} \left(\frac{1 \text{ mol S}}{32.1 \text{ g S}} \right) \left(\frac{1 \text{ mol Al}_2\text{S}_3}{3 \text{ mol S}} \right) = 0.156 \text{ mol Al}_2\text{S}_3 \quad \text{Limiting}$$

Sulfur is the limiting reagent.

$$0.156 \text{ mol Al}_2\text{S}_3 \left(\frac{150.3 \text{ g Al}_2\text{S}_3}{1 \text{ mol Al}_2\text{S}_3} \right) = 23.4 \text{ g Al}_2\text{S}_3$$

4. How much of the nonlimiting reactant is in excess in question 3?

$$0.156 \text{ mol Al}_2\text{S}_3 \left(\frac{2 \text{ mol Al}}{1 \text{ mol Al}_2\text{S}_3} \right) \left(\frac{27.0 \text{ g Al}}{1 \text{ mol Al}} \right) = 8.42 \text{ g Al used}$$

starting mass – mass used = mass remaining

$$10.0 \text{ g} - 8.42 \text{ g} = 1.6 \text{ g Al remaining}$$

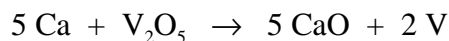
D) Yields of a reaction

Two types of yields

- 1) **actual yield**: quantity of product obtained from the reaction
- 2) **theoretical yield**: amount of product predicted when all the limiting reagent is used up.

$$\% \text{ yield} = \frac{\text{actual yield}}{\text{theoretical yield}} \times 100$$

Example:



In one process $1.54 \times 10^3 \text{ g}$ of V_2O_5 reacted with $1.96 \times 10^3 \text{ g}$ Ca

- a) Calculate the theoretical yield of vanadium.

In order to calculate the theoretical yield, the limiting reagent must be determined first.

$$1.54 \times 10^3 \text{ g V}_2\text{O}_5 \left(\frac{1 \text{ mol V}_2\text{O}_5}{181.88 \text{ g V}_2\text{O}_5} \right) \left(\frac{2 \text{ mol V}}{1 \text{ mol V}_2\text{O}_5} \right) = 16.9 \text{ mol V limiting}$$

$$1.96 \times 10^3 \text{ g Ca} \left(\frac{1 \text{ mol Ca}}{40.08 \text{ g Ca}} \right) \left(\frac{2 \text{ mol V}}{5 \text{ mol Ca}} \right) = 19.6 \text{ mol V}$$

The limiting reagent is V_2O_5 .

$$16.9 \text{ mol V} \left(\frac{50.94 \text{ g}}{1 \text{ mol V}} \right) = 863 \text{ g V}$$

The theoretical yield of vanadium is 863 g.

b) Calculate the percent yield of the above reaction if 803 g of V are obtained.

$$\frac{\text{actual yield}}{\text{theoretical yield}} \times 100 = \frac{803 \text{ g}}{863 \text{ g}} \times 100 = 93.0\%$$

III) Molarity and Dilutions

A) Molarity

Molarity is a concentration unit which gives the moles of solute in a liter of solution.

$$\text{Molarity} = \frac{\text{mol solute}}{\text{L solution}}$$

Example:

What is the molarity of the resulting solution when 45.00 g NaCl is placed into a 100 mL volumetric flask?

First convert the mass of the solute into moles.

$$5.35 \text{ g NaCl} \left(\frac{1 \text{ mol NaCl}}{58.45 \text{ g NaCl}} \right) = 0.0915 \text{ mol NaCl}$$

Next calculate the molarity.

$$\frac{\text{mol solute}}{\text{L solution}} = \frac{0.0915 \text{ mol NaCl}}{0.100 \text{ L solution}} = 0.915 \frac{\text{mol NaCl}}{\text{L}} = 0.915 \text{ M NaCl}$$

Molarity can be used as a conversion factor in solving problems.

example:

How many grams of NaCl are in 0.500 L of a 0.625 M NaCl solution?

$$\text{The given molarity is } 0.625 \text{ M NaCl} = \frac{0.625 \text{ mol NaCl}}{1 \text{ L solution}}$$

$$0.500 \text{ L} \left(\frac{0.625 \text{ mol NaCl}}{1 \text{ L}} \right) = 0.312 \text{ mol NaCl} \left(\frac{58.45 \text{ g NaCl}}{1 \text{ mol NaCl}} \right) = 18.3 \text{ g NaCl}$$

B) Dilutions

What happens during a dilution?

- solvent is added
- volume of the solution increases
- concentration of the solution decreases
- moles of the solute remains the same

Because the moles of solute remains constant during a dilution, a relationship between the old and new concentrations can be derived.

$$M = \frac{\text{mol solute}}{\text{L solution}} \quad \text{rearrange this definition to solve for moles of solute}$$

$$\begin{aligned} \text{mol solute} &= M \times (\text{L solution}) & \text{let } V &= \text{L solution} \\ \text{mol solute} &= M \times V \end{aligned}$$

The product the molarity and the volume gives the moles of solute in the solution.

$$\text{mol solute} = M_1 \times V_1 \quad \text{moles of solute at the initial molarity and volume}$$

$$\text{mol solute} = M_2 \times V_2 \quad \text{moles of solute at the final molarity and volume}$$

since the moles of solute remains constant during the dilution

$$M_1 \times V_1 = M_2 \times V_2$$

This relationship determines either the new volume or molarity of the diluted solution or the volume or molarity of the original solution.

Example:

A stock solution of NaCl is 6.00 M. How much of this stock solution is needed to prepare 1.00 L of physiological saline solution, which is 0.154 M NaCl?

$$M_1 V_1 = M_2 V_2$$

$$V_1 = \frac{M_2 V_2}{M_1} = \frac{(0.154 \text{ M})(1.00 \text{ L})}{(6.00 \text{ M})} = 0.0257 \text{ L} = 25.7 \text{ mL}$$

IV) Empirical Formulas

A) Mass percent from a chemical formula

The mass percentage of each element in a compound is the **percent composition**

$$\text{mass \% element} = \frac{\text{mass of element in compound}}{\text{mass of compound}} \times 100$$

Example:

Find the mass percentage of each element in ascorbic acid $\text{HC}_6\text{H}_7\text{O}_6$.

The molar mass of ascorbic acid is 176.1 g/mol

$$\% \text{ H} = \frac{(8)(1.01 \text{ g/mol})}{176.1 \text{ g/mol}} \times 100 = 4.59 \%$$

$$\% \text{ C} = \frac{(6)(12.0 \text{ g/mol})}{176.1 \text{ g/mol}} \times 100 = 40.9 \%$$

$$\% \text{ O} = \frac{(6)(16.0 \text{ g/mol})}{176.1 \text{ g/mol}} \times 100 = 54.5 \%$$

Perform a check: The mass percentages of each element should sum to 100 %

$$4.59 \% + 40.9 \% + 54.5 \% = 100.0 \%$$

B) Determining the empirical formula from the composition

Empirical formula is the smallest whole-number ratio of moles of each element in a compound.

Molecular formula shows all atoms in the compound.

name	empirical formula	molecular formula
hydrogen peroxide	HO	H_2O_2

Note: compounds can have the same empirical formulas but different molecular formulas.

Method for determining the empirical formula from the % composition
(finding the subscripts)

- 1) Assume 100.0 g of sample (unless given)
- 2) convert grams of each element into moles
- 3) the number of moles become the subscript in the chemical formula
- 4) divide subscripts by smallest (goal: whole number subscripts)
- 5) If any subscript is not an integer, then multiply all subscript by the smallest whole number to convert all subscripts into integers.

Example:

sodium pyrophosphate is used in detergent preps. The mass percentages of the elements in this compound are Na 34.6 %, P 23.3 %, O 42.1 %. What is the empirical formula of sodium pyrophosphate?

- 1) convert % composition into grams by assuming 100.0 g of sample

$$\text{Na: } 100 \text{ g } (0.346) = 34.6 \text{ g Na}$$

$$\text{P: } 100 \text{ g } (0.233) = 23.3 \text{ g P}$$

$$\text{O: } 100 \text{ g } (0.421) = 42.1 \text{ g O}$$

- 2) convert grams to moles

$$\text{Na: } 34.6 \text{ g Na} \left(\frac{1 \text{ mol Na}}{23.0 \text{ g Na}} \right) = 1.5 \text{ mol Na}$$

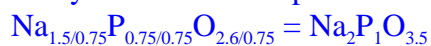
$$\text{P: } 23.3 \text{ g P} \left(\frac{1 \text{ mol P}}{31.0 \text{ g P}} \right) = 0.75 \text{ mol P}$$

$$\text{O: } 42.1 \text{ g O} \left(\frac{1 \text{ mol O}}{16.0 \text{ g O}} \right) = 2.6 \text{ mol O}$$

- 3) moles become subscripts



- 4) divide by smallest subscript



- 5) multiple by smallest whole number to convert all subscripts into integers



$\text{Na}_4\text{P}_2\text{O}_7$ is the empirical formula of sodium pyrophosphate

C) Determining the molecular formula from the empirical formula

To find the molecular formula to pieces of information is needed.

- 1) the molecular weight or molar mass of the compound
- 2) the **empirical weight** of the compound which is the sum of the atomic weights in the empirical formula

$$n = \frac{\text{molecular weight}}{\text{empirical weight}}$$

n is a whole number multiplier which converts the empirical formula into the molecular formula. n multiplies the subscripts in the empirical formula

Example:

Lactic acid forms in the muscles and is responsible for muscle soreness. Elemental analysis shows that lactic acid contains 40.0 % C, 6.71 % H, and 53.3 % O. The molar mass of this compound was found to be 90.08 amu.

- a) Determine the empirical formula of lactic acid.
- b) Determine the molecular formula of lactic acid.

a) assume 100 g of sample

$$\text{C: } 40.0 \text{ g C} \left(\frac{1 \text{ mol C}}{12.0 \text{ g C}} \right) = 3.33 \text{ mol C}$$

$$\text{H: } 6.71 \text{ g H} \left(\frac{1 \text{ mol H}}{1.0 \text{ g H}} \right) = 6.71 \text{ mol H}$$

$$\text{O: } 53.3 \text{ g O} \left(\frac{1 \text{ mol O}}{16.0 \text{ g O}} \right) = 3.33 \text{ mol O}$$



$$\text{empirical wt.} = 12.0 \text{ amu} + 2.0 \text{ amu} + 16.0 \text{ amu} = 30.0 \text{ amu}$$

$$\text{b) } n = \frac{90.08 \text{ amu}}{30.0 \text{ amu}} = 3$$



V) Quantitative analysis

A) Gravimetric analysis

Gravimetric analysis is a type of quantitative analysis in which the amount of a species in a material is determined by converting the species to a product that can be isolated completely and weighed.

Precipitation reactions are used often in gravimetric analyses.

Example:

A soluble silver compound was analyzed for the percentage of silver by adding sodium chloride solution to precipitate the silver ion as silver chloride. If 1.583 g of silver compound gave 1.788 g of AgCl, what is the mass % of Ag in the compound?

From the chemical formula, 1 mole of AgCl consists of 1 mol of Ag⁺ and 1 mol Cl⁻

$$1.788 \text{ g AgCl} \left(\frac{1 \text{ mol AgCl}}{143.4 \text{ g AgCl}} \right) \left(\frac{1 \text{ mol Ag}^+}{1 \text{ mol AgCl}} \right) \left(\frac{107.9 \text{ g Ag}^+}{1 \text{ mol Ag}^+} \right) = 1.345 \text{ g Ag}^+$$

$$\text{mass \%} = \frac{\text{mass of element}}{\text{mass of compound}} \times 100 = \frac{1.345 \text{ g}}{1.583 \text{ g}} \times 100 = 84.97 \% \text{ Ag}$$

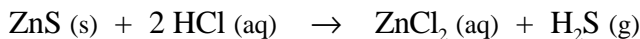
B) Volumetric analysis

Volumetric analysis is a method of analysis based on titration.

Titration is a procedure for determining the amount of substance A by adding a carefully measured volume of a solution with known concentration of B until the reaction of A and B is just complete.

Example:

Zinc sulfide reacts with hydrochloric acid to produce dihydrogen sulfide gas



How many mL of 0.0512 M HCl are required to react with 0.392 g ZnS?

$$0.392 \text{ g ZnS} \left(\frac{1 \text{ mol ZnS}}{97.5 \text{ g ZnS}} \right) \left(\frac{2 \text{ mol HCl}}{1 \text{ mol ZnS}} \right) \left(\frac{1 \text{ L HCl}}{0.0512 \text{ mol HCl}} \right) \left(\frac{10^3 \text{ mL}}{1 \text{ L}} \right) = 157 \text{ mL HCl sol'n}$$

recall that molarity can be used as a conversion factor to convert mole of a substance into volume.