Chapter 3 Calculations with Chemical Formulas and Equations

(Sections 3.1, 3.2, 4.3, and 4.4 in OpenStax)

Molar Masses (MM) and Avogadro's Number

- Molecular Mass or Weight (MM or MW) is the sum of the atomic masses for all of the atoms in a molecular compound, such as H_2O.
- Formula Mass or Weight (FM or FW) is similar, but the sum uses the formula unit of a non-molecular (ionic) compound, such as NaCl.
- A mole is the quantity of atoms in exactly 12 g of ^{12}C, which is Avogadro's number.

  Avogadro's number: $N_A = 6.022 \times 10^{23} \frac{\text{amu}}{\text{g}}$ (or $\frac{\text{molecules}}{\text{mole}}$)

  This quantity represents a mole for all atoms, molecules, and formula units.
- N_A allows us to convert between amu and g so that

  Molar Mass in $\left(\frac{\text{g}}{\text{mole}}\right)$ = Molar Mass in $\left(\frac{\text{amu}}{\text{atom}}\right)$

Ex 3.01 Determine the Molar Mass of a Molecular Compound (H_2O)

$$\left(\frac{2\text{ H atoms}}{1\text{ H}_2\text{O molecule}} \times 1.01 \frac{\text{amu}}{\text{H atom}}\right) + \left(\frac{1\text{ O atom}}{1\text{ H}_2\text{O molecule}} \times 16.00 \frac{\text{amu}}{\text{O atom}}\right) = 18.02 \frac{\text{amu}}{\text{H}_2\text{O molecule}} \left(\text{or } \frac{\text{g}}{\text{mole}}\right)$$

Ex 3.02 Determine the Molar Mass of a Nonmolecular Compound (NaCl)

$$\left(\frac{1\text{ Na atom}}{1\text{ NaCl unit}} \times 22.99 \frac{\text{amu}}{\text{Na atom}}\right) + \left(\frac{1\text{ Cl atom}}{1\text{ NaCl unit}} \times 35.45 \frac{\text{amu}}{\text{Cl atom}}\right) = 58.44 \frac{\text{amu}}{\text{NaCl unit}} \left(\text{or } \frac{\text{g}}{\text{mole}}\right)$$

Ex 3.03 Determine the Mass of one Sodium (Na) atom using N_A as a Conversion Factor

$$\left(\frac{22.99\text{ g}}{1\text{ mole Na}}\right) \times \left(\frac{1\text{ mole Na}}{6.022 \times 10^{23}\text{ Na atoms}}\right) = 3.818 \times 10^{-23} \frac{\text{g}}{\text{Na atom}}$$

Ex 3.04 Convert 0.0524 moles of iron(III) bromide into grams

- The molar mass of $FeBr_3$ is

  $$\left(\frac{1\text{ mole Fe}}{1\text{ mole FeBr}_3} \times 55.85 \frac{\text{g}}{\text{mole Fe}}\right) + \left(\frac{3\text{ moles Br}}{1\text{ mole FeBr}_3} \times 79.90 \frac{\text{g}}{\text{mole Br}}\right) = 295.55 \frac{\text{g}}{\text{mole FeBr}_3}$$
- The mass of $FeBr_3$ is $0.0524\text{ mol FeBr}_3 \times \left(\frac{295.55\text{ g}}{1\text{ mole FeBr}_3}\right) = 15.5\text{ g}$

Ex 3.05 Convert 25.4 grams of iron(II) sulfate into moles

- The molar mass of $FeSO_4$ is 1(Fe) + 1(S) + 4(O) = 55.85 + 32.07 + 4(16.00) = 151.92 g/mol
- The number of moles is $25.4\text{ g} \times \left(\frac{1\text{ mol}}{151.92\text{ g}}\right) = 0.167\text{ mol}$

Ex 3.06 Determine the number of Chlorine (Cl_2) molecules using N_A as a Conversion Factor

- The molar mass of Cl_2 is $\frac{2\text{ moles Cl}}{1\text{ mole Cl}_2} \times 35.45 \frac{\text{g}}{\text{mole Cl}} = 70.90 \frac{\text{g}}{\text{mole Cl}_2}$
- $(100.0\text{ g of Cl}_2) \times \left(\frac{1\text{ mole Cl}_2}{70.90\text{ g}}\right) \times \left(\frac{6.022 \times 10^{23}\text{ molecules}}{1\text{ mole}}\right) = 8.49 \times 10^{23}$ molecules of Cl_2

Mass Percentages of Elements in a Compound

- Mass % of a component = $\left[\frac{\text{mass of component in compound}}{\text{total mass of compound}}\right] \times 100\%$

Ex 3.07 Find the Mass %'s of carbon, hydrogen, and oxygen in formaldehyde

- The molar mass of CH_2O is 12.01 + 2(1.01) + 16.00 = 30.03 g/mol
- The component masses in one mole of CH_2O are:

  $C = \left(\frac{\text{1 mole C}}{\text{1 mole } CH_2O}\right) \times \left(\frac{\text{12.01 g of C}}{\text{1 mole C}}\right) = 12.01\ \frac{\text{g of C}}{\text{1 mole } CH_2O}$

  $H = \left(\frac{\text{2 mole H}}{\text{1 mole } CH_2O}\right) \times \left(\frac{\text{1.01 g of H}}{\text{1 mole H}}\right) = 2.02\ \frac{\text{g of H}}{\text{1 mole } CH_2O}$

  $O = \left(\frac{\text{1 mole O}}{\text{1 mole } CH_2O}\right) \times \left(\frac{\text{16.00 g of O}}{\text{1 mole O}}\right) = 16.00\ \frac{\text{g of O}}{\text{1 mole } CH_2O}$

- Divide the component mass of each element by the molar mass of the compound.

  $\% C = \frac{\text{12.01 g of C}}{\text{30.03 g } CH_2O} \times 100\ \% = 40.0\ \%$

  $\% H = \frac{\text{2.02 g of H}}{\text{30.03 g } CH_2O} \times 100\ \% = 6.7\ \%$

  $\% O = \frac{\text{16.00 g of O}}{\text{30.03 g } CH_2O} \times 100\ \% = 53.3\ \%$

- This means 100.0 g of CH_2O will contain 40.0 g of C, 6.7 g of H, and 53.3 g of O.

Ex 3.08 Determine the mass of C in a 124.5 g sample of CH_2O

$(124.5\text{ g } CH_2O) \times \left(\frac{\text{40.0 g of C}}{\text{100.0 g of CH2O}}\right) = 49.8\text{ g of C}$

Total Carbon and Hydrogen Analysis (See Figure)

- $C_nH_mO_q$ is combusted with O_2 to create nCO_2 and $\left(\frac{m}{2}\right)H_2O$
- Masses of CO_2 and H_2O created are converted into masses of C and H with a similar method to examples 3.07 and 3.08 by using mass ratios: $\left(\frac{\text{12.0 g C}}{\text{44.0 g CO2}}\right)$ and $\left(\frac{\text{2.02 g H}}{\text{18.02 g H2O}}\right)$
- After subtracting masses of C and H from the sample mass, the remaining mass, if any, in the sample is due to O.
- The masses of C, H, and O are each divided by the overall sample mass to find the mass %'s in the sample.
- The elements' mass %'s are divided by their atomic masses to convert them into moles for each element. The moles can then be used those to find the compound's empirical formula.

Empirical Formula

- Written with the smallest possible set of integer subscripts.
- Same as formula unit for most ionic compounds (except those with Hg_2^{+2}).
- But is not necessarily same as formula for molecular compounds.
- C_2H_2 (acetylene) and C_6H_6 (benzene) both have the same empirical formula: CH.

Ex 3.10 Determine the Empirical Formula from the Element Masses

- 1.127 g of a nitrogen oxide has 0.343 g N and 0.784 g O
- $(0.343 \text{ g N}) \times \left(\frac{1 \text{ mole N}}{14.0 \text{ g}}\right) = 0.0245 \text{ mol N}$ $\quad (0.784 \text{ g O}) \times \left(\frac{1 \text{ mole O}}{16.0 \text{ g}}\right) = 0.0490 \text{ mol O}$
- $\frac{\text{moles O}}{\text{moles N}} = \frac{0.0490}{0.0245} = 2.00 \text{ mol O per mol N}$
- The empirical formula is NO_2. So, the compound can be NO_2 or N_2O_4.

Ex 3.11 Determine the Empirical Formula from the Element Mass Percentages

- Potassium dichromate is 26.6 % K, 35.3 % Cr, and 38.1 % O by mass.
- That means 100.0 g potassium dichromate has 26.6 g K, 35.3 g Cr, and 38.1 g O
- $(26.6 \text{ g K}) \times \left(\frac{1 \text{ mol K}}{39.1 \text{ g}}\right) = 0.680 \text{ mol K}$ $\quad \frac{0.680}{0.680} = 1.000$
- $(35.3 \text{ g Cr}) \times \left(\frac{1 \text{ mol Cr}}{52.0 \text{ g}}\right) = 0.679 \text{ mol Cr}$ $\quad \frac{0.679}{0.680} = 0.999 \approx 1$
- $(38.1 \text{ g O}) \times \left(\frac{1 \text{ mol O}}{16.0 \text{ g}}\right) = 2.38 \text{ mol O}$ $\quad \frac{2.38}{0.680} = 3.50$
- Double those numbers to get all integer values: $K_2Cr_2O_7$

Relating empirical formula mass to molecular mass

- For molecular compounds, MM is an integer multiple of empirical formula mass
- $n = \frac{\text{molecular mass}}{\text{empirical formula mass}}$

Ex 3.12 Determine the Molecular Formula from the Molar Mass and the Empirical Formula

- Acetic acid's element mass %'s are 39.9 % C, 6.7 % H, and 53.4 % O.
- The moles of C, H, and O in 100 g of acetic acid as follows:

$$(39.9 \text{ g C}) \times \left(\frac{1 \text{ mole C}}{12.0 \text{ g}}\right) = 3.33 \text{ moles C}$$

$$(6.7 \text{ g H}) \times \left(\frac{1 \text{ mole H}}{1.01 \text{ g}}\right) = 6.6 \text{ moles H}$$

$$(53.4 \text{ g O}) \times \left(\frac{1 \text{ mole O}}{16.0 \text{ g}}\right) = 3.34 \text{ moles O}$$

- Divide those results by 3.33 to get the empirical formula, which is CH_2O.
- The empirical formula mass of CH_2O = 12.01 + 2(1.01) + 16.00 = 30.03 g/mol
- The molar mass of acetic acid can be determined with a mass spectrometer.

  MM = 60.06 g/mol = (n)(30.03 g/mol) and n = 2
- The actual molecular formula is $(CH_2O)_2 = C_2H_4O_2$ (or CH_3COOH).

Stoichiometry

- Stoichiometry is the calculation of quantities of reactants and products involved in a chemical reaction.
- The reaction equation can use either molecules or moles as units. The ratios for the substances are the same, regardless of which units are used.

  1 molecule N_2 + 3 molecules H_2 $\rightarrow$ 2 molecules NH_3

  or 1 mole N_2 + 3 moles H_2 $\rightarrow$ 2 moles NH_3
- If the equation is in moles, then we can convert the moles into masses.

  (1 mole N_2) × (28.0 g/mol) = 28.0 g N_2

  (3 moles H_2) × (2.02 g/mol) = 6.06 g H_2

  (2 moles NH_3) × (17.03 g/mol) = 34.06 g NH_3
- Moles are proportional to stoichiometric coefficients. So, we can use the coefficients to create a conversion factor, and then find the amount of H_2 needed to create 4.20 mol NH_3.

  $$(4.20 \text{ mol NH}_3 \text{ created})\left(\frac{3 \text{ mol H}_2}{2 \text{ mol NH}_3}\right) = 6.30 \text{ moles H}_2 \text{ needed}$$
- We can find the mass of H_2 needed to create 1 metric ton (1000 kg) of NH_3 by using that same conversion factor along with conversions between moles and masses.

  First, convert to moles of NH_3: $$(1000 \text{ kg})\left(\frac{1000 \text{ g}}{1 \text{ kg}}\right)\left(\frac{1 \text{ mol NH}_3}{17.0 \text{ g}}\right) = 5.88 \times 10^4 \text{ moles NH}_3$$

  Then, find the moles of H_2: $$(5.88 \times 10^4 \text{ moles NH}_3)\left(\frac{3 \text{ mol H}_2}{2 \text{ mol NH}_3}\right) = 8.82 \times 10^4 \text{ moles H}_2$$

  Finally, convert to mass of H_2: $$(8.82 \times 10^4 \text{ moles H}_2)\left(\frac{2.02 \text{ g H}_2}{\text{mol}}\right) = 1.78 \times 10^5 \text{ g H}_2$$

  $$1.78 \times 10^5 \text{ g H}_2 \times \left(\frac{1 \text{ kg}}{10^3 \text{ g}}\right) = 178 \text{ kg H}_2$$

Ex 3.13 Use Stoichiometry to Determine the Mass of Al Product

- In the Hall-Héroult process, aluminum is created from aluminum oxide and carbon.

  $$2Al_2O_{3(s)} + 3C_{(s)} \rightarrow 4Al_{(s)} + 3CO_{2(g)}$$
- Mole ratios can be used to determine the Al mass that can be created from 1000 g of Al_2O_3.
- Convert mass of reactant into moles: $$(1000 \text{ g Al}_2\text{O}_3)\left(\frac{1 \text{ mol Al}_2\text{O}_3}{101.96 \text{ g}}\right) = 9.808 \text{ moles Al}_2\text{O}_3$$
- Convert to moles of product: $$(9.808 \text{ moles Al}_2\text{O}_3)\left(\frac{4 \text{ mol Al}}{2 \text{ mol Al}_2\text{O}_3}\right) = 19.62 \text{ mol Al}$$
- Convert moles of product into mass: $$(19.62 \text{ mol Al})\left(\frac{26.98 \text{ g}}{1 \text{ mol Al}}\right) = 529.3 \text{ g Al}$$

Limiting Reactant

- A substance that will be entirely consumed by a complete reaction is limiting.
- A substance that cannot be entirely consumed by a complete reaction is present in excess.
- The maximum moles of product possible are determined by the starting moles of the limiting reactant.

Ex 3.15 Finding the Amount of H_2 Product Possible from the Limiting Reactant

- $Mg_{(s)} + 2HCl_{(aq)} \rightarrow MgCl_{2(aq)} + H_{2(g)}$
- Suppose we have 0.640 mol Mg and 0.820 mol HCl.
- $(0.640 \text{ mol Mg}) \times \left(\frac{1 \text{ mol } H_2}{1 \text{ mol Zn}}\right) = 0.640 \text{ mol } H_2$
- $(0.820 \text{ mol HCl}) \times \left(\frac{1 \text{ mol } H_2}{2 \text{ mol HCl}}\right) = 0.410 \text{ mol } H_2$
- HCl is the limiting reactant because it makes the lesser amount of H_2. Only 0.410 moles of H_2 are produced when the reaction is complete.
- Once 0.410 moles of H_2 are created, there will be no HCl left, and the reaction stops.
- Some excess Mg will remain present after the HCl is consumed and the reaction stopped.
- The mass of H_2 produced in a complete reaction is $(0.410 \text{ mol } H_2)(2.02 \text{ g/mol}) = 0.828 \text{ g}$

Theoretical Yield

- The theoretical yield is the maximum amount of product that can be obtained from a complete reaction.
- It is the maximum amount of product produced when the limiting reactant has been completely consumed.
- In Ex 3.15 above, the theoretical yield of H_2 is 0.410 mol or 0.828 g.

Actual Yield

- The actual yield is usually less than the theoretical yield for several reasons.
  - Products or reactants can escape or be lost.
  - Other competing reactions can deplete reactants.
  - Reactions typically stop before 100% completion.

Percent Yield

- $\text{Percent Yield} = \left[\frac{(\text{Actual Yield})}{(\text{Theoretical Yield})}\right] \times 100\%$
- Suppose the theoretical yield is 0.828 g (0.410 mol) of H_2, and the actual yield is 0.722 g.

  $\text{Percent yield} = \left(\frac{0.722 \text{ g actual}}{0.828 \text{ g theoretical}}\right) \times 100\% = 87.2\%.$
- The same value will be found if the units are in moles instead of g (because units cancel).

  $(0.722 \text{ g}) \times \left(\frac{1 \text{ mole } H_2}{2.02 \text{ g}}\right) = 0.35\underline{7}4 \text{ moles } H_2$

  $\text{Percent Yield} = \left(\frac{0.3574 \text{ moles actual}}{0.410 \text{ moles theoretical}}\right) \times 100\% = 87.2\%$