Reactions can be categorized as Physical or Chemical

Physical reactions occur when a substance transitions from one physical state to another (e.g. water boiling)

* There is <u>NOT</u> a change in the molecule, <u>ONLY</u> intermolecular interactions

$$H_2O_{(l)} \rightarrow H_2O_{(g)}$$

Subscripts indicate phase
s = solid, l = liquid, g = gas
aq = aqueous

Chemical reactions occur when the atomic composition of a molecule changes

$$\underbrace{2Na_{(s)} + Cl_{2(g)}}_{\text{Reactants}} \rightarrow \underbrace{2NaCl_{(s)}}_{\text{Products}}$$

Rules for writing chemical reactions (or physical reactions):

① Physical states must be shown

② matter must be conserved

↳ If you have 2 Na atoms in your reactants, you <u>must</u> have 2 in the products

Balancing chemical reaction:

$$4Al + 3O_2 \rightarrow 2Al_2O_3$$

Al	$\cancel{1}$ 4		$\cancel{2}$ 4
O		$\cancel{2}$ 6	$\cancel{3}$ 6

$$C_3H_{4(g)} + 4O_{2(g)} \rightarrow 3CO_{2(g)} + 2H_2O_{(l)}$$

C	3		$\cancel{1}$ 3	
H	4			$\cancel{2}$ 4
O		$\cancel{2}$ 8	$\cancel{2}$ 6	$\cancel{1}$ 2 = 8

$$2Na_{(s)} + 2H_2O_{(l)} \rightarrow 2NaOH_{(aq)} + H_{2(g)}$$

Na	$\cancel{1}$ 2 ✓		$\cancel{1}$ 2 ✓	
H		$\cancel{2}$ 4 ✓	$\cancel{1}$ 2	2 = 4 ✓
O		$\cancel{1}$ 2 ✓	$\cancel{1}$ 2 ✓	

You should be comfortable converting verbal descriptions of chemical reactions to a chemical equation

Solid Phosphorus reacts with oxygen to form Tetraphosphorus decaoxide solid

$$4P_{(s)} + 5O_{2(g)} \rightarrow P_4O_{10}\,(s)$$

Types of chemical reactions:

Synthesis: $X + Y \rightarrow Z$ $\quad CO_2(g) + H_2O(l) \rightarrow H_2CO_3(aq)$

two or more compounds react to form one

Decomposition: $Z \rightarrow X + Y$ $\quad 2ZnO_{(s)} \rightarrow 2Zn(s) + O_2(g)$

- opposite of synthesis
- one compound breaks apart to form two or more new compounds

Single Replacement $XY + Z \rightarrow X + ZY$ $\quad Na_{(s)} + KCl_{(aq)} \rightarrow K_{(s)} + NaCl_{(aq)}$

- one component of a binary compound exchanges with a monoatomic molecule } commonly ion exchange

Double Replacement $AB + XY \rightarrow AY + BX$ $\quad NaCl + KBr \rightarrow NaBr + KCl$

- Cations in ionic compounds switch place

Combustion $C_xH_y + zO_2 \rightarrow xCO_2 + \frac{y}{2}H_2O$ $\quad CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$

- Hydrocarbon reacts with molecular oxygen; CO_2 & H_2O are produced

So for the rest of this class, we'll be focusing on chemical reactions. One MAJOR thing that chemists need to do on a regular basis is to predict how much product will form given certain amounts of reactants

But here is the catch: masses of reactants and products are NOT directly related

For example:

$$Na + KCl \rightarrow NaCl + K$$

excess, so we won't run out

If we start with 1.00 g $Na_{(s)}$ and excess KCl, there is NO straight forward way to calculate the amount of NaCl will be produced

We could use the number of atoms:

10 Na atom will produce 10 NaCl molecules

* but we don't have a good way to measure atoms *
- only mass is measurable

- So we're going to introduce a new unit that allows us to relate atoms to grams

– the mole –

Conceptually, a mole is absolutely no different than a dozen

1 dozen = 12 units

I you have 2 dozen donuts, how many donuts?

$$\frac{2 \text{ dozen}}{} \Big| \frac{12 \text{ donuts}}{1 \text{ dozen}} = 24 \text{ donuts}$$

36 cars → how many dozen?

$$\frac{36 \text{ cars}}{} \Big| \frac{1 \text{ dozen}}{12 \text{ cars}} = 3 \text{ dozen}$$

Treat moles the same way: (Just a much bigger number)

$$1 \text{ mol} = 6.022 \times 10^{23} \text{ units}$$

46 moles of donuts → how many donuts?

$$\frac{46 \text{ mol}}{} \Big| \frac{6.022 \times 10^{23} \text{ donuts}}{1 \text{ mol}} = 2.77 \times 10^{25} \text{ donuts}$$

1×10^{20} atoms of carbon. How many moles?

$$\frac{1 \times 10^{20} \text{ atoms}}{} \Big| \frac{1 \text{ mol}}{6.022 \times 10^{23}} = 1.66 \times 10^{-4} \text{ mol}$$

Since moles are <u>DIRECTLY</u> related to number of atoms, we can use this unit to relate atoms & molecules to other atoms/molecules

If I have 4.5 moles of Carbon Dioxide: ① How many moles of carbon?

② How many moles of Oxygen?

③ How many of each atom?

① We can use the subscripts in CO_2 as conversion factors:

$1 \text{ mol } CO_2 = 1 \text{ mol Carbon}$

$$\frac{4.5 \text{ mol } CO_2 \mid 1 \text{ mol C}}{\mid 1 \text{ mol } CO_2} = 4.5 \text{ mol Carbon}$$

② $$\frac{4.5 \text{ mol } CO_2 \mid 2 \text{ mol O}}{\mid 1 \text{ mol } CO_2} = 9 \text{ mol Oxygen}$$

$$\frac{4.5 \text{ mol Carbon} \mid 6.022 \times 10^{23} \text{ atoms}}{\mid 1 \text{ mol}} = 2.71 \times 10^{24} \text{ atoms carbon}$$

$$\frac{9 \text{ mol O} \mid 6.022 \times 10^{23} \text{ atoms}}{\mid 1 \text{ mol}} = 5.42 \times 10^{24} \text{ atoms oxygen}$$

We can also use the mol unit to relate the amount of products and reactants in a chemical reaction:

Stoichiometric coefficient

$$MgO + 2NaCl \rightarrow MgCl_2 + Na_2O$$

If I have 10 moles of MgO and excess NaCl, how much $MgCl_2$ can we produce?

- use the stoichiometric as a conversion factor: $1 \text{ mol } MgO = 1 \text{ mol } MgCl_2$

$$\frac{10 \cancel{\text{ mol MgO}} \mid 1 \text{ mol } MgCl_2}{\mid 1 \cancel{\text{ mol MgO}}} = 10 \text{ mol } MgCl_2$$

What if we have 10 moles of NaCl and excess MgO, how much $MgCl_2$ will be produced

$$\frac{10 \text{ mol NaCl} \mid 1 \text{ mol } MgCl_2}{\mid 2 \text{ mol NaCl}} = 5 \text{ mol } MgCl_2$$

Since it takes 2 moles of NaCl to produce 1 mol of $MgCl_2$, we only get 5 moles

But... we cannot measure moles or atoms! We CAN measure mass

One of the most important conversions we'll see this term

g ⟶ mol   This conversion factor comes from the periodic table.

- The average isotopic mass of an element (e.g. Carbon is 12.011) has the unit $\frac{\text{grams}}{1\text{ mol}}$. This is the Molecular Weight

Molar mass
Atomic mass
Atomic weight

- these terms tend to be used interchangeably. The most correct one highlighted

moles can be calculated from the mass of a substance using the molecular weight

How many moles of carbon are present in 1.00 g?   MW = 12.011 g/mol (from periodic table)

$$\frac{1.00\text{ g C}}{} \left| \frac{1\text{ mol}}{12.011\text{ g}} \right. = 0.0833\text{ mol C}$$

How many carbon atoms?

$$\frac{0.0833\text{ mol C}}{} \left| \frac{6.022\times10^{23}\text{ atoms}}{1\text{ mol}} \right. = 5.01\times10^{22}\text{ atoms}$$

16.82 g CO_2 → How many grams of oxygen?

CO_2 → MW = 12.011 + 2(16.) = 44.011 g/mol   * need to go through moles! *

$$\frac{16.82\text{ g }CO_2}{} \left| \frac{1\text{ mol }CO_2}{44.011\text{ g }CO_2} \right| \frac{2\text{ mol O}}{1\text{ mol }CO_2} \left| \frac{16\text{ g}}{1\text{ mol O}} \right. = 12.23\text{ g Oxygen}$$

Class Problem:

Using the chart to aid in calculations.

Consider CH_4. If you are told that you have 172 grams of carbon in CH_4, how many atoms (H & C) exist in this sample?

Strategy: There are several ways to tackle this problem. My approach is to recognize that there are 4 Hydrogens for every 1 carbon. If we are able to determine how many C atoms, we can determine H

mass C → moles C → atoms C → atoms H → total atoms

$$\frac{172 \text{ g C}}{} \left| \frac{1 \text{ mol C}}{12.011 \text{ g C}} \right| \frac{6.022 \times 10^{23} \text{ atoms}}{1 \text{ mol}} = 8.62 \times 10^{24} \text{ C atoms}$$

$$\frac{8.62 \times 10^{24} \text{ C atoms}}{} \left| \frac{4 \text{ H atoms}}{1 \text{ C atom}} \right. = 3.45 \times 10^{25} \text{ H atoms}$$

$$8.62 \times 10^{24} + 3.45 \times 10^{25} = 4.31 \times 10^{25}$$

Now calculate the mass of CH_4 which contains 172 g Carbon

Strategy: mass C → moles C → mol CH_4 → mass CH_4

$$\frac{172 \text{ g C}}{} \left| \frac{1 \text{ mol C}}{12.011 \text{ g C}} \right| \frac{1 \text{ mol } CH_4}{1 \text{ mol C}} \left| \frac{16.05 \text{ g } CH_4}{1 \text{ mol } CH_4} \right. = 229.86 \text{ g } CH_4$$

IN 229.86 grams of CH_4, carbon accounts for 172 g

The % → $\frac{172}{229.86} \times 100 = 74.83\%$

Mass % → The percentage of a molecule's mass that comes from one atom

Elemental analysis data is MUCH more common in the form of mass %

this is JUST a conversion factor!

CO_2 is 72.71% oxygen by mass. If you have 42.86 g CO_2, what mass of oxygen?

$$\frac{72.71 \text{ g oxygen}}{100 \text{ g } CO_2}$$

$$\frac{42.86 \text{ g } CO_2}{} \left| \frac{72.71 \text{ g O}}{100 \text{ g } CO_2} \right. = 31.16 \text{ g oxygen}$$

Calculating mass% → these are just mole conversions!

What is the mass% C in $C_2H_4O_2$?

Let's assume 100g $C_2H_4O_2$.

$$\text{mass \%} = \frac{X}{100\,g\,C_2H_4O_2} \times 100$$

X = mass C in 100g $C_2H_4O_2$ ← 12.01(2) + 4(1.01) + 2(16)

24.02 4.04 32

60.06 g/mol

$$\frac{100\,g\,C_2H_4O_2}{} \left| \frac{1\,mol\,C_2H_4O_2}{60.06\,g} \right| \frac{2\,mol\,C}{1\,mol\,C_2H_4O_2} \left| \frac{12.01\,g}{1\,mol} \right. = 39.96\,g\,C$$

$$\frac{39.96\,g\,C}{100\,g\,C_2H_4O_2} \times 100 = 39.96\%$$

Now calculate H + O

H: 7.19% O: 53.28%

How else can we use mol conversions? Determining molecular Formulas!

First, we need to categorize compound formulas:

Molecular Formula: the exact atomic composition of a molecule

Empirical Formula: The lowest possible ratio of atoms in a compound

Molecular Formula	Empirical Formula
CO_2 →	CO_2
C_2O_4 →	CO_2
C_3H_6 →	CO_2

Lots of compounds can have the same Empirical Formula!

Decomposition of a sample reveals that it is composed of: 3.6 g Carbon

0.61 g Hydrogen

4.8 g Oxygen

① Determine the Empirical Formula.

② Determine the molecular formula if this compound has a MW = 90.09

① 1. convert to moles

2. Divide by lowest number of moles

3. divide by lowest decimal again if necessary.

this assumes that at least one atom has a coeff. of 1

$$C: \frac{3.6\,g\,C}{} \left| \frac{1\,mol}{12.01\,g} \right. = \frac{0.2998\,mol\,C}{0.2998} = 1\,mol\,C$$

$$H: \frac{0.61\,g\,H}{} \left| \frac{1\,mol}{1.01\,g} \right. = \frac{0.604\,mol\,H}{0.2998} = 2.01\,mol\,H$$

$$O: \frac{4.8\,g\,O}{} \left| \frac{1\,mol}{16.\,g} \right. = \frac{0.3\,mol\,O}{0.2998} = 1\,mol\,O$$

$\boxed{CH_2O}$

② - Determine MW of Empirical Formula — $12.01 + 2(1.01) + 16 = 30.03$ g/mol

- Since E.F. is M.F. ÷ an integer, this is also true for M.W.

$$\frac{\text{M.W.}}{\text{E.F.W.}} = n \qquad \frac{90.09}{30.03} = 3$$

E.F.W. ← Empirical Formula Weight

E.F = CH_2O ← 3×

Molecular Formula = $C_3H_6O_2$

Molecular Formula vs. Empirical Formula

$\underbrace{\text{Molecular Formula}}_{\text{actual formula}}$ vs. $\underbrace{\text{Empirical Formula}}_{\text{Lowest integer ratio of atoms}}$

$C_6H_6 \rightarrow$ E.F. = CH

$C_2H_3 \rightarrow$ E.F. = C_2H_3

$C_8H_{18} \rightarrow$ E.F. = C_4H_9

This E.F. is useful because it lets us quickly determine the identity of a compound from experimental data!

- Elemental analysis determines that a compound contains 24.27 g Carbon, 4.075 g Hydrogen + 71.65 g Chlorine. and has a molecular weight of 98.96 g/mol

* mass is NOT relatable → convert to moles! *

$$\frac{24.27\text{ g C}}{} \left| \frac{\text{mol}}{12.01\text{ g}} \right. = \frac{2.02\text{ mol C}}{2.02} = 1$$

$$\frac{4.075\text{ g H}}{} \left| \frac{1\text{ mol}}{1.01\text{ g}} \right. = \frac{4.03\text{ mol H}}{2.02} = 2$$

$$\frac{71.65\text{ g Cl}}{} \left| \frac{1\text{ mol}}{35.45\text{ g}} \right. = \frac{2.02}{2.02} = 1$$

E.F. = CH_2Cl

$2(1.01) + 12.01 + 35.45$

E.F.W. = 49.48 g/mol

$$\frac{MW}{EFW} = \text{number of times the Molecule formula is bigger than the empirical formula} = \frac{98.96}{49.48} = 2$$

$\boxed{C_2H_4Cl_2}$

Consider Trifluoroacetic acid:

$$21.6\%\ C \left| \frac{\text{mol}}{12.011\text{ g}} \right. = \frac{1.75}{0.876} = 2 \qquad 49.9\%\ F \left| \frac{\text{mol}}{19\text{ g}} \right. = \frac{2.63}{0.876} = 3$$

$$0.89\%\ H \left| \frac{\text{mol}}{1.01\text{ g}} \right. = \frac{0.876}{0.876} = 1 \qquad 28.06\%\ O \left| \frac{\text{mol}}{16\text{ g}} \right. = \frac{1.75}{0.876} = 2$$

$\boxed{HC_2F_3O_2}$