CHEM1011 LECTURE 3

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REMINDER

Labs start next week!

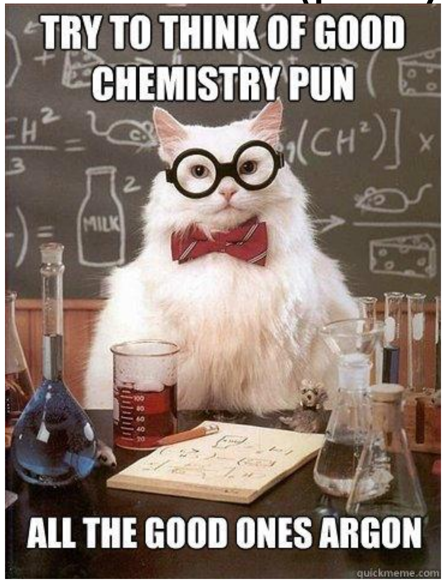
Know when and where your class is (a good start)

Read and watch the pre lab material and complete the pre lab safety and calculation exercises.

Wear enclosed shoes, safety glasses and a lab coat!

Be on time! if you are more than 20 mins late you will not be allowed in (plus you will miss all the important stuff)

Don't be like this

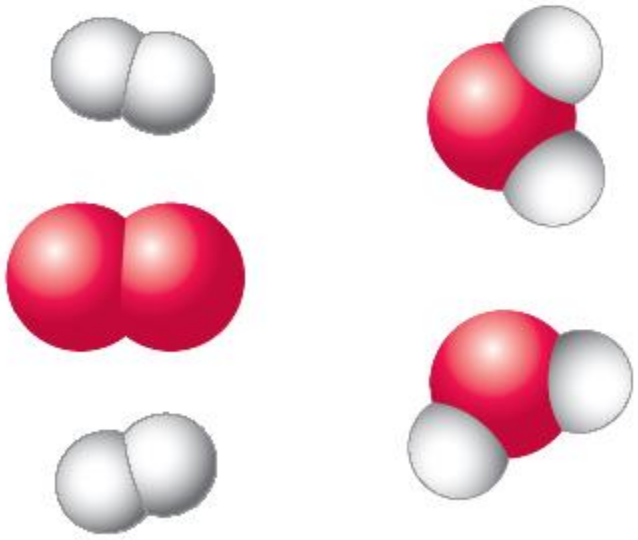


Be like this

CHEMICAL EQUATIONS

- **Stoichiometry** is concerned with the relative amounts of reactants and products in a chemical reaction *(Law of multiple proportions).*

- **Stoichiometric coefficients** indicate the simplest ratio of molecules, ions or atoms among the reactants and products.



$$2H_2 + O_2 \longrightarrow 2H_2O$$

PARTS OF A CHEMICAL EQUATION

Chemical species.

$$1\,P_4\,(s) + 5\,O_2\,(g) \longrightarrow 1\,P_4O_{10}\,(s)$$

Coefficients

State symbols

- In balancing an equation the numbers <u>within</u> each chemical species CAN NOT be changed. This would be changing the identities of the chemicals involved.

- Coefficients can be changed to balance the equation.

- State symbols tell the physical state of the species, which can affect the reaction rate, and its energy change.

CHEMICAL EQUATIONS - STATES OF MATTER

Specifying states of matter

- It is useful to specify the physical states of the reactants and products.
- This is done by writing:
  - (s) for solid,
  - (l) for liquid or
  - (g) for gas after the chemical formula
  - (aq), meaning ‘aqueous solution’, is used to indicate that a particular substance is dissolved in water.

You are expected to do this whenever writing equations in chem1011

CHEMICAL EQUATIONS

- The law of conservation of mass says that atoms cannot be created or destroyed during a chemical reaction.
- Stoichiometric coefficients are used to balance an equation to meet this condition.

2 molecules of C_4H_{10} | 13 molecules of O_2 | 8 molecules of CO_2 | 10 molecules of H_2O

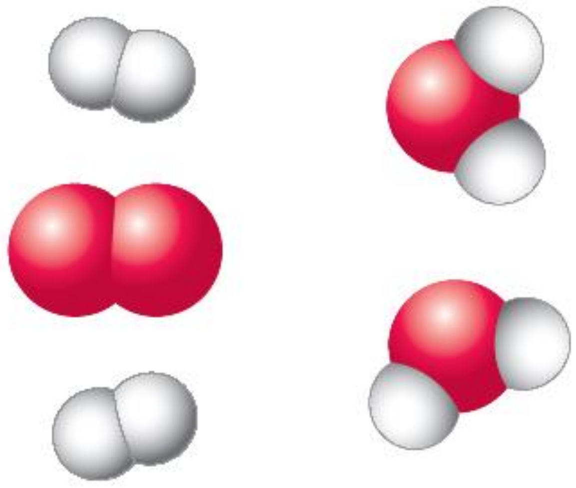
$$\boxed{2C_4}H_{10} + 13O_2 \longrightarrow 8CO_2 + 10H_2O$$

How many C atoms?

CHEMICAL EQUATIONS

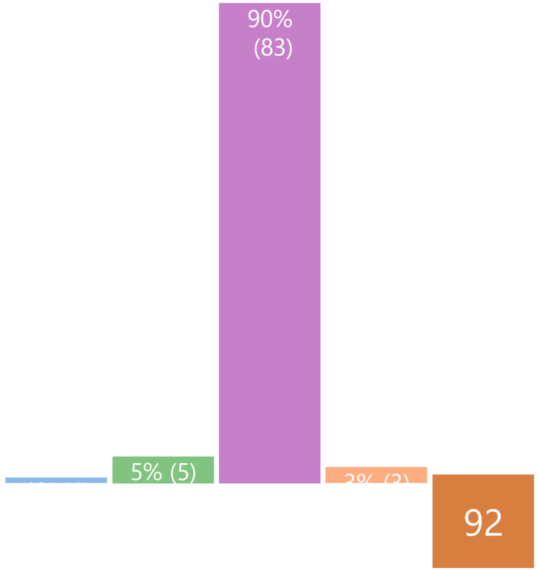
- **Stoichiometry** is concerned with the relative amounts of reactants and products in a chemical reaction
- **Stoichiometric coefficients** indicate the simplest ratio of molecules, ions or atoms among the reactants and products

What is the stoichiometric ratio of H_2 : H_2O in this reaction?



$$2H_2 + O_2 \longrightarrow 2H_2O$$

- A 1:2
- B 2:2
- C 1:1 ✓
- D 2:1



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EQUATIONS AND STOICHIOMETRY

Blackman 3.3

Stoichiometry - ratio in which chemical species react - the coefficients of species in a balanced chemical equation. (relative number of atoms).

Knowing the mass of 1 atom (in amu) is not so useful…how can we count lots of atoms by weighing them instead??

Use the MOLE - the chemists ‘dozen’.

Avogadro constant (6.0231×10^{23} mol^{-1}) gives the number of entities in 1 mole.

EQUATIONS AND STOICHIOMETRY

Blackman 3.3

A mole of a substance is the mass of it, in grams, that contains the same number of entities as there are in exactly 12.000 g of carbon-12

The weight of a mole of a substance is its atomic or molecular mass expressed in grams.

Atomic mass in amu is equal to the mole mass in grams

i.e 1 Mo atom weighs 95.94 amu

1 mole of Mo atoms weighs 95.94g

The mole (abbreviated mol) is the SI unit of **amount of substance**

MOLE

A mole in chemistry is:

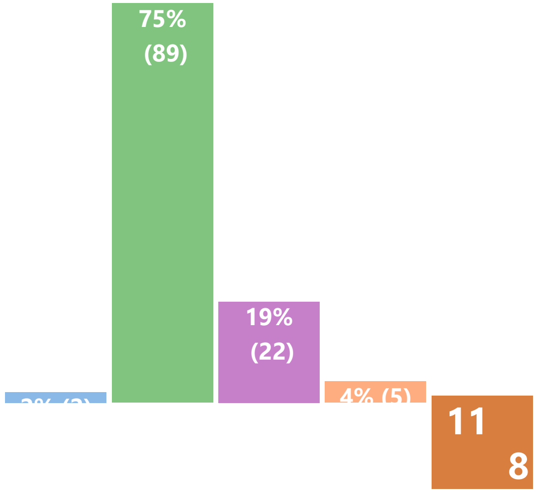
A A molecule that has been broken down into its constituent parts

B A unit (mol)

C The number 6.022×10^{23}

D

https://upload.wikimedia.org/wikipedia/commons/8/87/Mr_Mole.jpg



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INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

A NEW DEFINITION OF THE MOLE HAS ARRIVED

8 January 2018

After an extensive consultation with the chemistry community, and following a review and critical evaluation of the literature, IUPAC is recommending a new definition of the mole based on a specified number of elementary entities:

> The mole, symbol mol, is the SI unit of amount of substance. One mole contains exactly $6.022\,140\,76 \times 10^{23}$ elementary entities. This number is the fixed numerical value of the Avogadro constant, N_A, when expressed in mol^{-1}, and is called the Avogadro number.

Responding to the announcement of the new definition, Professor Peter W. Atkins, founding Chair of IUPAC Committee on Chemistry Education, commented as followed: “I have always been puzzled by the widespread view that the mole is a difficult subject: it has always seemed to me that many instructors tell their students that it is a sophisticated concept, and the students then wonder what all the fuss is about, suspecting that they have misunderstood it or have not appreciated its subtlety. The new definition cuts to the core of the meaning of 1 mole, and is therefore to be welcomed. Although there are subtleties in its determination, there can no longer be any excuse for misunderstanding its definition.”

https://iupac.org/new-definition-mole-arrived/

THE MOLE – MOLAR MASS

- The molar mass, M, is the mass of 1 mole of a substance

- What is the molar mass of water (H_2O)?
  - The chemical formula tells us it is made up of 2 hydrogen atoms and 1 oxygen atom
  - Hence the molar mass is the sum of twice the atomic mass of hydrogen (1.008 g) plus the atomic mass of oxygen (15.999 g)
  - $M_{H_2O} = (2 \times 1.008 \text{ g}) + 15.999 \text{ g} = 18.015 \text{ g}$

– The relationship between amount of substance (moles, n), molar mass (M) and mass (m) is given by $M = m/n$
– Commonly used as $n = m/M$

MOLECULAR MASS

Molecular masses are found by summing atomic masses of the component atoms.

$$\text{Amount of A (in moles)} = \frac{\text{actual mass of A}}{\text{molar (molecular) mass}}$$

$$n = \frac{m}{M}$$

e.g. Amount of H_2O in 1000 g of water = $\dfrac{1000\ \text{g}}{18\ \text{g mol}^{-1}}$

= <u>55.6 mole</u>

Note: Formula mass of ionic compounds

- use its empirical formula.
- e.g. 1 mole of NaCl = 22.99 + 35.45 = <u>58.44 g mol^{-1}</u>

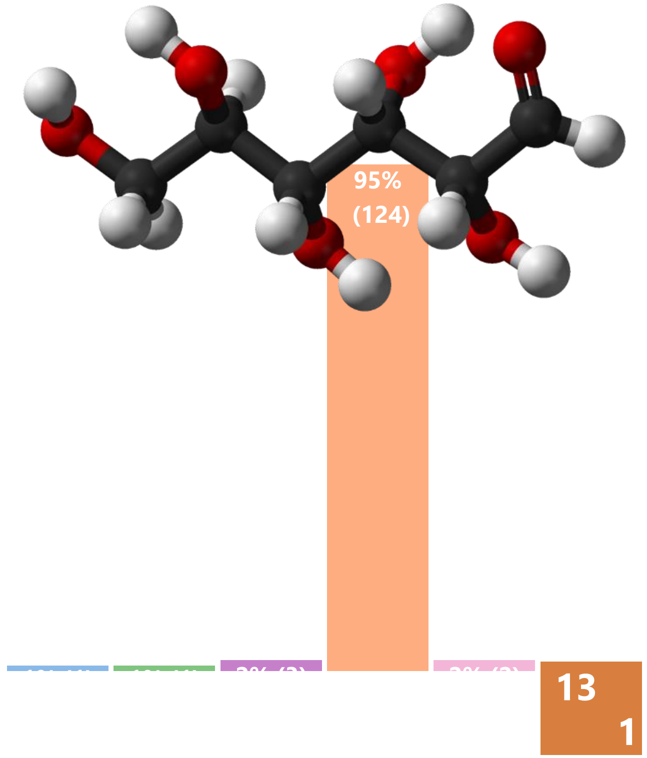
2 decimal places recommended!

1 H 1.008	6 C 12.01	7 N 14.01	8 O 16.00

MOLAR MASS

The molar mass of glucose ($C_6H_{12}O_6$) is ______________ g/mol?

- A 29.018
- B 30.026
- C 180
- ✓ D 180.16
- E Don't know



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WRITING AND BALANCING CHEMICAL EQUATIONS

GUIDE FOR WRITING EQUATIONS

- Write reactants on left, products on right (by convention).
- Include states of matter.
- Change coefficients to give the same count for each element on both sides. (do not change subscript numbers) this is called balancing: (Leave H and O until last)
  1. Balance elements that appear in one species on both sides,
  2. Balance elements that appear in several species on both sides.
  3. Balance H atoms
  4. Balance O atoms
- For reactions in water you may add H_2O if needed to balance oxygen atoms.
- For reactions in water, you may add H^+ if needed to balance hydrogen atoms if requires.
- Give nett ionic equations if possible – convey essential change by removing the spectator ions.

FROM WORDS TO BALANCED EQUATIONS

You need to know formula, name translations, and the nature of solutions, to change a description into a chemical equation.

- Hydrochloric acid reacts with solid sodium hydroxide to produce a sodium chloride solution and water.
- Aluminium sulfate solution and calcium nitrate solution are reacted to give a precipitate of calcium sulfate and a solution of aluminium nitrate.
- Solid sodium oxide reacts with water to give a sodium hydroxide solution.
- Manganese dioxide reacts with lead dioxide when heated in suspension in acidic water, to give permanganate ions and lead ions.

EQUATIONS AND STOICHIOMETRY- WORKED EXAMPLE

" solid sodium hydroxide is reacted with hydrochloric acid to produce a sodium chloride solution and water".

Re-expressing names as chemical species:

Hydrochloric acid is HCl(aq), which contains H^+(aq) + $Cl^–$(aq)

Solid sodium hydroxide is NaOH(s), which contains Na^+ ions and $OH^–$ ions packed close together in the crystals.

Sodium chloride solution contains Na^+(aq) ions and $Cl^–$(aq) ions.

$$H^+(aq) + Cl^–(aq) + NaOH(s) \rightarrow Na^+(aq) + Cl^–(aq) + H_2O(l)$$

Nett equation: $H^+(aq) + NaOH(s) \rightarrow Na^+(aq) + H_2O(l)$

EQUATIONS AND STOICHIOMETRY

"aluminium sulfate solution and calcium nitrate solution are reacted to give a precipitate of calcium sulfate and a solution of aluminium nitrate."

$$Al^{3+}(aq) \; + \; SO_4^{2-}(aq) \; + Ca^{2+}(aq) \; + NO_3^{-}(aq) \; \rightarrow CaSO_4(s) \; + Al^{3+}(aq) + NO_3^{-}(aq))$$

Nett: $Ca^{2+}(aq) + SO_4^{2-}(aq) \;–> CaSO_4(s)$

EQUATIONS AND STOICHIOMETRY

"Solid sodium oxide reacts with water to give a sodium hydroxide solution."

$$Na_2O(s) \quad + H_2O(l) \quad \text{–>} \; 2 \; Na^+(aq) \; + \; 2 \; OH^-(aq)$$

YOU TRY!

A solution of barium nitrate is mixed with a solution of potassium carbonate leading to the formation of a white precipitate of barium carbonate

barium nitrate => $Ba(NO_3)_2$

solution => $Ba^{2+}(aq)$ and 2 $NO_3^-(aq)$

potassium carbonate => K_2CO_3

solution => 2 $K^+(aq)$ and $CO_3^{2-}(aq)$

YOU TRY!

A solution of barium nitrate is mixed with a solution of potassium carbonate leading to the formation of a white precipitate of barium carbonate

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solution => $Ba^{2+}(aq)$ and $2\ NO_3^-(aq)$

potassium carbonate => K_2CO_3

solution => $2\ K^+(aq)$ and $CO_3^{2-}(aq)$

1.include only the ions which undergo a change in state i.e. (aq) to (s)

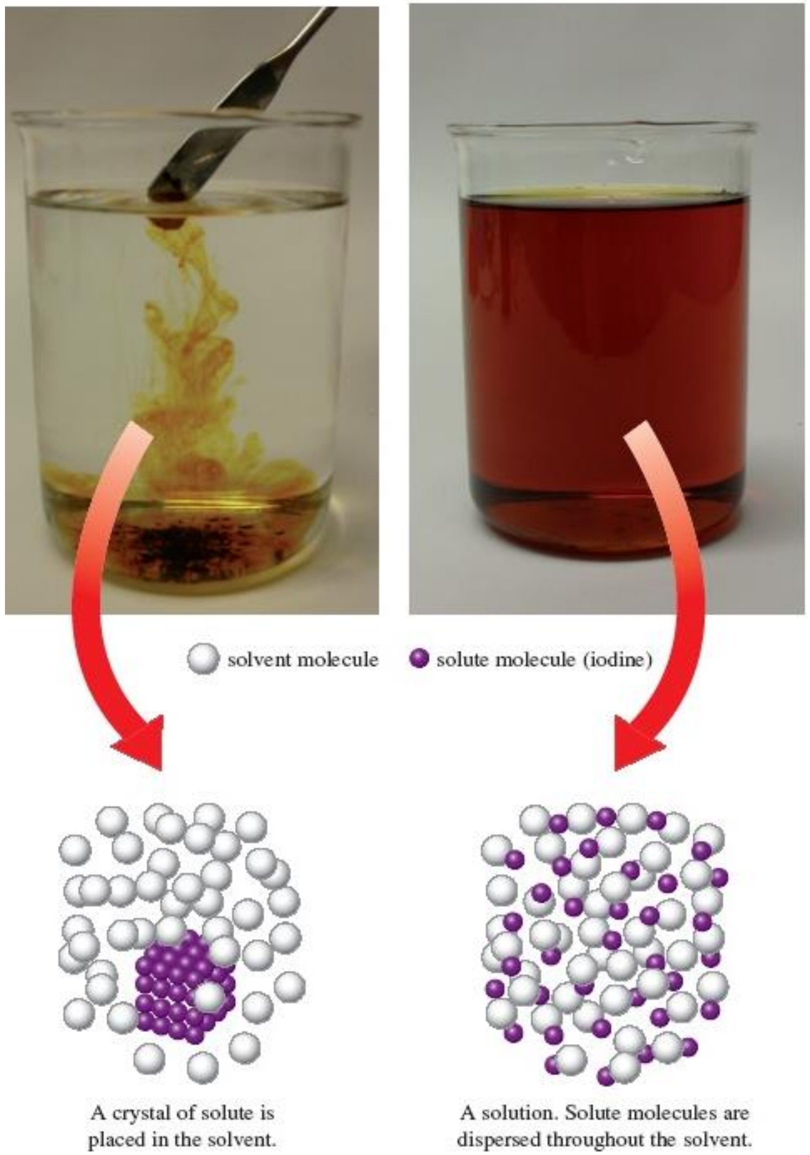
2. Show the change of state by including the state symbols

$$Ba^{2+}(aq) + CO_3^{2-}(aq) \rightarrow BaCO_3\,(s)$$

CHEMICAL SOLUTIONS

SOLUTION STOICHIOMETRY (BLACKMAN 3.6)

- Chemical reactions are nearly always carried out in solution to allow mixing
- A solution is a homogeneous mixture
- When a solution forms, at least two substances are involved, a solvent and one or more solutes
- The solvent is the component present in largest amount
- The solute is any substance dissolved in the solvent

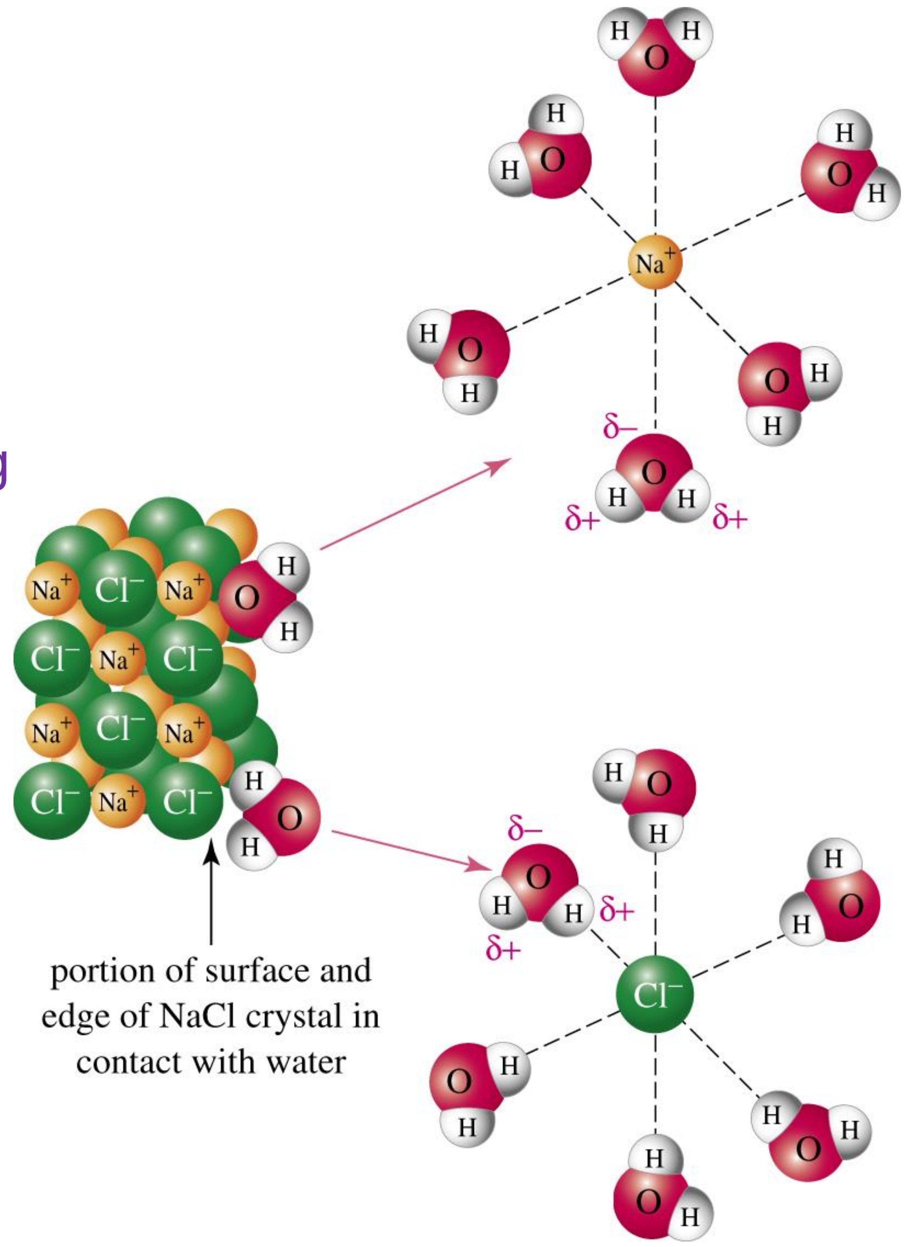


What are Ions in Water ?

In an **ionic solid**, the ions bond together strongly, owing to their opposite charges (e.g. Na^+ and Cl^-).

Ionic solids dissolve in water because the breaking of ion-ion attractions of the solid is compensated for by H_2O molecules forming strong bonds to each individual ion (solvation).

Also favouring dissolving: ions in solution can move randomly in the bigger volume of liquid (increased randomness).



SOLUTION STOICHIOMETRY - MOLARITY

The concentration of solutions

- The concentration is most often defined as the amount of solute dissolved in a particular volume of solution.
- The concentration of a substance X is represented as [X]   i.e. in square brackets [ ] i.e $[Na^+] = 0.2$ M
- When the amount is given in moles and the volume in litres, it is called the molarity or molar concentration : mol L^{-1}

SOLUTION STOICHIOMETRY

- Molarity (or molar concentration) has the units mol L^{-1} (often abbreviated M)
- Concentration is based on the ratio of the amount of solute to the volume of solution
- The equation defining concentration is:

The units of c are mol L^{-1}

$$C = \frac{n}{V}$$

n is the number of moles

V is the volume (in Litres)

OTHER METHODS OF DEFINING SOLUTION STOICHIOMETRY (BLACKMAN 10.5)

Molarity

- Amount of substance in a particular volume of solution
- Solutions (usually) increase in volume with increasing temperature
- The molarity of a solution changes as the temperature changes
- Can create problems

- Three other methods of defining stoichiometry that do not depend on volume and so are temperature independent are molality (note spelling), mole fraction and percentage composition by mass.

MOLE FRACTION

- The number of moles of a particular component divided by the total number of moles of material in the solution

- The mole fraction of *A*, X_A, in a solution containing substances *A*, *B* and *C:*

$$\boxed{X_A = \frac{n_A}{n_A + n_B + n_C}}$$

- Temperature independent

- Sum of mole fractions for all components = 1

PERCENTAGE COMPOSITION BY MASS- BLACKMAN 3.4

- The relative masses of components of a solution (or elements in a compound) may be given as a percentage
- This is called the percentage composition OR percentage composition by mass
- The percentage by mass of a components is calculated using the following:

$$\% \text{ component} = \frac{\text{mass of component}}{\text{mass of whole sample}} \times 100\%$$

EQUATIONS AND STOICHIOMETRY

Measures of Concentration Summary:

Mass %

$$\text{mass \%} = \frac{\text{mass of solute}}{\text{mass of solution}} \times \frac{100}{1} \ \%$$

Mole Fraction

$$X_A = \frac{\text{moles of A}}{\text{moles of (A + B + ...)}}$$

Note that $X_A + X_B = 1$ for a 2 component system.

Molarity

$$\text{Molarity} = \frac{\text{moles of solute}}{\text{litres of solution}} \quad \text{(Molar)}$$

Units: M or mol L^{-1}

DILUTIONS

Calculate the volume of concentrated reagent required to make the following dilution:

18.0 M H_2SO_4 to make 5.0L of 5.0M H_2SO_4

$$\boxed{C = \frac{n}{V}}$$

$$\boxed{C_1V_1 = C_2V_2}$$

This formula is valid ONLY for dilutions

DILUTIONS

Calculate the volume of concentrated reagent required to make the following dilution:

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This formula is valid ONLY for dilutions

Dilutions involve taking a volume of concentrated solution (an *aliquot*) and making it up to a set volume with water. The number of moles of the solute in the aliquot of concentrated solution is therefore the same as the number of moles in the diluted solution.

Hence we can use this formula to determine the volume the more concentrated aliquot must be to prepare the prescribed diluted solution.

DILUTIONS

$$C = \frac{n}{V}$$

$$C_1V_1 = C_2V_2$$

This formula is valid ONLY for dilutions

Calculate the volume of concentrated reagent required to make the following dilution:

$\boxed{18.0\ M}_{C_1}$ H_2SO_4 to make $\boxed{5.0L}_{V_2}$ of $\boxed{5.0M}_{C_2}$ H_2SO_4

1.The question is asking us to determine the volume of the aliquot needed to make the dilution, i.e. V_1

2.Because we know the number of moles in the aliquot of the concentrated solution = moles in diluted solution we can use the dilution formula.

We rearrange the formula to solve for V_1 i.e. $V_1 = C_2V_2/C_1 = 5.0 \times 5.0 / 18 = 1.39L = 1.4L$ (lowest number s.f)

UNSW SYDNEY

SOLUTION STOICHIOMETRY

- Ionic compounds dissociate into their constituent ions when dissolved in water
- This can have important consequences in stoichiometric calculations
  - e.g. $CaBr_2$ undergoes complete dissociation into Ca^{2+} and Br^- ions, according to the equation

$$CaBr_2(s) \rightarrow Ca^{2+}(aq) + 2Br^{-}(aq)$$

  - 0.10 moles of $CaBr_2$ yields 0.10 moles of Ca^{2+} and 0.20 moles of Br^-
  - In 0.10M $CaBr_2$, the concentration of Ca^{2+} is 0.10 M and the concentration of Br^- is 0.20 M

YOU TRY

For each of the following solutions?

1. Write the dissolution equation.

2. determine the stoichiometric ratio between product and reactants.

3. give the concentration for each ion in solution.

1.2 M $Ba(NO_3)_2$

0.5 M $Al_2(SO_4)_3$

YOU TRY

For each of the following solutions?

1. Write the dissolution equation.
2. determine the stoichiometric ratio between product and reactants.
3. give the concentration for each ion in solution.

1.2 M $Ba(NO_3)_2$

$Ba(NO_3)_2(s) \rightarrow Ba^{2+}(aq) + 2NO_3^-(aq)$

1 : 1 : 2

Using the ratios $Ba(NO_3)_2$: Ba^{2+} = 1:1 so $[Ba^{2+}]$ =$[Ba(NO_3)_2]$ = 1.2M

$Ba(NO_3)_2$: NO_3^- = 1:2 so $[NO_3^-$ =2 $[Ba(NO_3)_2]$ = 2.4M

YOU TRY

For each of the following solutions?

1. Write the dissolution equation.
2. determine the stoichiometric ratio between product and reactants.
3. give the concentration for each ion in solution.

0.5 M $Al_2(SO_4)_3$

$Al_2(SO_4)_3(s) \rightarrow 2Al^{3+}(aq) + 3SO_4^{2-}(aq)$

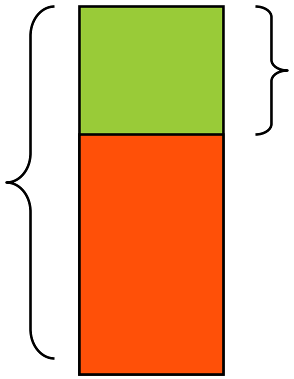
1 : 2 : 3

Using the ratios $Al_2(SO_4)_3 : Al^{3+} = 1:2$ so $[Al^{3+}] = 2\,[Al_2(SO_4)_3] = 1.0M$

$Al_2(SO_4)_3 : SO_4^{2-} = 1:3$ so $[SO_4^{2-}] = 3\,[Al_2(SO_4)_3] = 1.5M$

EXTENDED EXAMPLE

A concentrated solution of NH_3 in water contains 256 g of NH_3 per litre of solution; the solution has a density of 0.880 g ml^{-1}.
Calculate the molarity, mole fraction and % by mass of NH_3 in the solution.



% by mass:

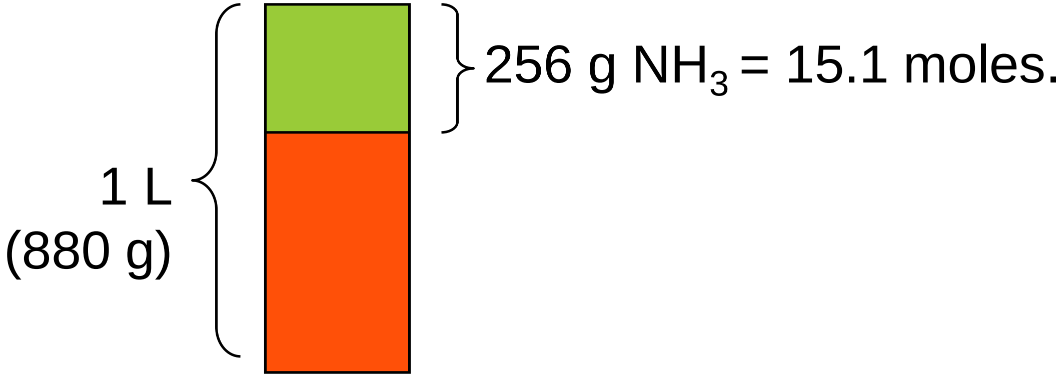
Consider 1 litre of the solution:

Its density is 0.880 g ml^{-1} , so 1000 ml of solution must weigh 880 g.

In this 1 litre of solution are 256 g of NH_3.
$\therefore$% of NH_3 in solution = (256g/880g) x 100 = 29.0 %.

(Continued …)

EXAMPLE Continued …



Molarity of NH_3 :

In the 1 litre of the solution are 256 g of NH_3

$$n = m/M$$

Moles NH_3 = 256/(14.01 + 3(1.008)) = 15.06 moles.

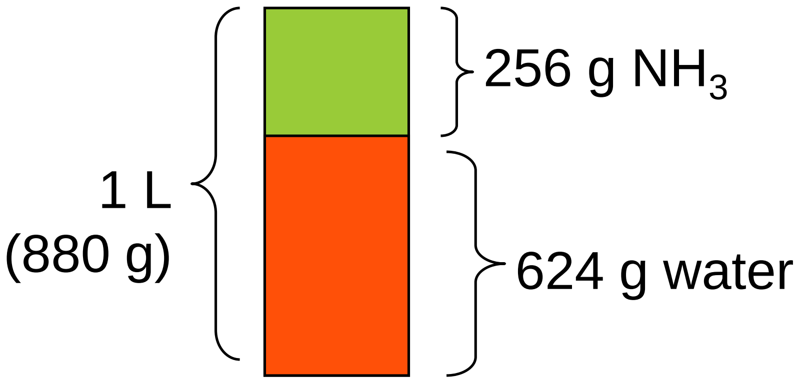
∴ molarity of NH_3 = 15.1 mole L^{-1}.

EXAMPLE Continued …

Note:

If 256 g of the 1000 ml of solution (weighing 880g) is NH_3, then the remaining weight is water, = 880g – 256g = 624 g.

We can use this knowledge in further calculations…



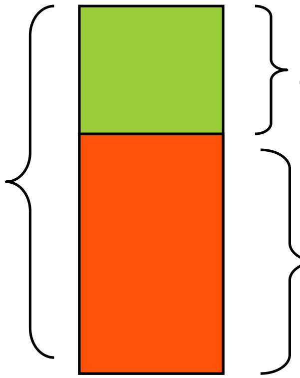
EXAMPLE Continued …

Mole fraction of NH_3 :

The 1 litre of solution contains 256 g (15.06 moles) of NH_3 and 624 g of water. This = (624 g/18 g mol^{-1}) = 34.67 mole of water.

Total moles of all species in 1 litre = 15.06 + 34.67 = 49.73 moles.

X_{NH_3} =(moles NH_3/moles of all components) = 15.06/49.73 = 0.303.



1 L
(880 g)

256 g NH_3 = 15.06 moles

624 g H_2O = 34.67 moles

TOTAL = 49.73 moles

Equations and Stoichiometry:

You try:

1. An aqueous solution containing 571.6 g of H_2SO_4 per litre of solution at 20° C has a density of 1.329 g cm^{-3}.

   Find the mass %, mole fraction and molarity of H_2SO_4 in the solution.

2. A sample of hydrochloric acid contains 40% HCl by mass. The density of the solution is 1.20 g cm^{-3}.

   What is the molarity of HCl in this solution?

LIMITING REAGENTS

LIMITING REAGENTS

What do you do if you really want cake but…..disaster!

You only have 25g of cocoa??

CHOCOLATE CAKE

INGREDIENTS

- Unsalted butter 175 gm
- Caster sugar 275 gm
- Eggs 2
- Vanilla essence 1 tbsp
- Sour cream 1/2 cup
- Flour 200 gm
- Soda bicarbonate 1/2 tsp
- Cocoa powder 50 gm
- Hot water 125 ml

METHOD

1. Preheat oven to 180 degree C and line tin.
2. In bowl, beat together butter, sugar, eggs, sour cream and essence till smooth.
3. Fold in flour, bicarb and cocoa, with a rubber spatula along with pouring boiling water.
4. Pour this batter into prepared tin and bake for 40 minutes.
5. Put cocoa, water and sugar into small saucepan and boil for 5 minutes till sugar caramelizes and syrup has a really dark n thick consistency.
6. Cool cake on cooling rack and, till in its tin and pierce with a cake tester.

EQUATIONS AND STOICHIOMETRY- LIMITING REAGENTS

What if we react chemicals in a non-stoichiometric ratio?

One of the reagents will be present in excess.

The moles of the other reagent will determine the maximum moles of product that can be formed, if it all reacts. This reagent is called the '<u>limiting reagent</u>'.

	$Fe (s)$ +	$S (s)$ –>	$FeS (s)$
Atom/species ratio:	1	1	1
Weight atoms :	55.85 amu	32.06 amu	87.91 amu
Ideal molar masses:	55.85 g	32.06 g	87.91 g
Reaction mixture:	55.85 g	38.0 g	0.0 g
After reaction:	0.0 g	5.94 g	87.91 g
	Limiting Reagent.	Excess Reagent.	

Given the following equation:

$Al_2(SO_3)_3 + 6\ NaOH \text{ ------> } 3\ Na_2SO_3 + 2\ Al(OH)_3$

a) If 10.0 g of $Al_2(SO_3)_3$ is reacted with 10.0 g of NaOH, determine the limiting reagent

b) Determine the number of moles of $Al(OH)_3$ produced

c) Determine the number of grams of Na_2SO_3 produced

d) Determine the number of grams of excess reagent left over

Given the following equation:

$Al_2(SO_3)_3$ + 6 NaOH ------> 3 Na_2SO_3 + 2 $Al(OH)_3$

a) If 10.0 g of $Al_2(SO_3)_3$ is reacted with 10.0 g of NaOH, determine the limiting reagent

First red flag is that we are given amounts of reactants in mass (g) but we can only compare the number of molecules (as per stoichiometric ratios in equation) so we need to translate to moles.

We know that n = m/M and we can derive the molecular mass (M) from the chemical formulae and periodic table.

M($Al_2(SO_3)_3$) = 294.15g/mol M(NaOH) = 40g/mol

n($Al_2(SO_3)_3$) = 10/294.15 = <u>0.034 mols</u> n(NaOH) = 10/40 = <u>0.25 mols</u>

It is not sufficient to just compare the two values of moles. We must consider them in the context of chemical reaction taking place and thus the stoichimetirc ratio.

In the equation above, the ratio of $Al_2(SO_3)_3$: NaOH = 1:6

Thus we need to consider if all of one of the reactants were to be used, how much of the other would be required….

Lets consider a scenario where all of the $Al_2(SO_3)_3$ is used. How many moles of NaOH would be required?

nNaOH: n$Al_2(SO_3)_3$ = 6:1 thus nNaOH = 6 n$Al_2(SO_3)_3$ so in this case n$Al_2(SO_3)_3$ = 0.034mols

So nNaOH required = 6 x 0.034 = 0.204 mols

How do we know which is the limiting reagent? We if we use ALL of the $Al_2(SO_3)_3$ as outlined above then we only use 0.204 mols of NaOH but we calculated that we actually have 0.25mols of NaOH

<u>Therefore $Al_2(SO_3)_3$ must be the limiting reagent</u> because we have excess NaOH when all $Al_2(SO_3)_3$ is used.

Given the following equation:

$Al_2(SO_3)_3$ + 6 NaOH ------> 3 Na_2SO_3 + 2 $Al(OH)_3$

b) Determine the number of moles of $Al(OH)_3$ produced

c) Determine the number of grams of Na_2SO_3 produced

From a) we know that we are reacting exactly 0.034 mols of $Al_2(SO_3)_3$ (the limiting reagent)

Using the stoichiometric ratio of $Al_2(SO_3)_3$ to the products we can determine the expected number of moles of each product.

b) $nAl(OH)_3$:$nAl_2(SO_3)_3$ = 2:1 therefore, $nAl(OH)_3$ = 2 $nAl_2(SO_3)_3$ = 0.034 x 2 = <u>0.068 mols</u>

c) nNa_2SO_3:$nAl_2(SO_3)_3$ = 3:1 therefore, nNa_2SO_3 = 3 $nAl_2(SO_3)_3$ = 0.034 x 3 =<u>0.102 mols</u>

Given the following equation:

$Al_2(SO_3)_3 + 6\ NaOH \text{ ------> } 3\ Na_2SO_3 + 2\ Al(OH)_3$

d) Determine the number of grams of excess reagent left over

From a) we determine both the nNaOH we had before the reaction and nNaOH that would be used up. Thus the left over reagent can be determined as the difference between these two values.

From a) before reaction :n(NaOH) = 10/40 = 0.25 mols

nNaOH used in reaction = 6 x 0.034 = 0.204 mols

Therefore remaining nNaOH = 0.25 – 0.204 = <u>0.046 mols</u>

However the question asks for the grams so we need to convert moles to mass

m = n.M = 0.046 x 40 = <u>1.84 g of NaOH remaining</u>

PERCENTAGE YIELD

STOICHIOMETRY, LIMITING REAGENTS AND PERCENTAGE YIELD (BLACKMAN 3.5)

Percentage yield

- In most experiments, the amount of a product isolated falls short of the maximum amount.
- The actual yield of the desired product is simply how much is isolated.
- The theoretical yield of the product is what would be obtained if no losses occurred.
- The percentage yield is the actual yield calculated as a percentage of the theoretical yield.

STOICHIOMETRY, LIMITING REAGENTS AND PERCENTAGE YIELD (BLACKMAN 3.5)

- Percentage yield is calculated using the following formula:

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

  - The calculation may be done in either grams or moles, but both yields must be in the same units
  - The actual yield can never be more than the theoretical yield

PERCENTAGE YEILD

Dichlorine monoxide, Cl_2O is sometimes used as a powerful chlorinating agent in research. It can be produced by passing chlorine gas over heated mercury (II) oxide according to the following equation:

$HgO + Cl_2 \rightarrow HgCl_2 + Cl_2O$

What is the percent yield, if the quantity of the reactants is sufficient to produce 0.86g of Cl_2O but only 0.71 g is obtained?

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What is the percent yield, if the quantity of the reactants is sufficient to produce 0.86g of Cl_2O but only 0.71 g is obtained?

This is a pretty straight forward application of the % yield formula as we are given the expected yield (what stoichiometric calculations suggest should be the amount made) and the actual yield (how much of the product was actually isolated from the reaction). This calculation can be done comparing wither masses or moles.. As long as you are comparing the same units.

% yield = actual yield/ expected yield x 100 = 0.71/0.86 x 100 = <u>61.1% (3s.f)</u>

PERCENTAGE YIELD – MORE COMPLEX

In the commercial production of the element arsenic, arsenic(III) oxide is heated with carbon, which reduces the oxide to the metal according to the following equation:

$2As_2O_3 + 3C \rightarrow 3CO_2 + 4As$

- If 8.87g of As_2O_3 is used in the reaction and 5.33 g of As is produced, what is the percent yield?

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This is a little more complicated because we are not given the expected yield of the As. However because we are given the amount of reactant that is used (As_2O_3), it is easy enough to use stoichiometry to calculate the expected yield of As.

First: Red flag, we are given masses but we can only use moles to compare in stoichiometric ratios so need to translate.

Thus n As_2O_3 used = m/M M As_2O_3 = 197.84g/mol, thus n As_2O_3 = 8.87/ 197.84g = <u>0.0448 mols</u>

To calculate the expected yield of As we need to compare the stoichiometric ratio of nAs: nAs_2O_3 = 4:2 =2:1 Thus nAs = 2n As_2O_3 = 2 x 0.0448 = <u>0.0897 mols</u>

Finally, we can't compare our expected and actual yield because they are in different units. So we will convert our expected yield into grams using m =nM ($M_{(As)}$ = 74.92 g/mol) m_{As} = 0.0897 x 74.92 = <u>6.72g</u>

Thus to complete the questions we need to place our expected and actual yield masses into the % yield formula

% yield = actual yield/ expected yield x 100 = 5.33/6.72 x 100 = <u>79.3%</u>

MOLECULAR FORMULA FROM EMPIRICAL FORMULA

EMPIRICAL FORMULAE (BLACKMAN 3.4)

- The empirical formula is the simplest whole-number ratio of atoms within that compound.

- For example, butane has the formula:

C_4H_{10} molecular formula

  – However this isn't the simplest ratio as both 4 and 10 are divisible by 2. Hence butane has the empirical formula:

C_2H_5 empirical formula

EMPIRICAL FORMULAE (BLACKMAN 3.4)

- The relative masses of elements in a compound is usually given as a percentage
- This is called the percentage composition OR percentage composition by mass
- The percentage by mass of an element is calculated using the following:

$$\% \text{ element} = \frac{\text{mass of element}}{\text{mass of whole sample}} \times 100\%$$

EMPIRICAL FORMULAE (BLACKMAN 3.4)

- A molecular formula gives the chemical composition of 1 molecule, e.g. P_4O_{10}.

- The empirical formula for this compound is P_2O_5.

- This gives the simplest whole number ratio between atoms.

- The empirical formula of a compound can be obtained experimentally by determining the mass of each element in a compound.

EMPIRICAL FORMULAE (BLACKMAN 3.4)

There are three steps necessary to determine the empirical formula:

1. Assume we are studying 100 g of the compound and therefore individual mass percentages become the actual masses
2. Convert the ratio of elements by mass to a ratio by amount, by dividing the mass of each element by its molar mass
3. Divide the resulting numbers by the smallest, which will give the smallest whole-number ratios of each element

EMPIRICAL FORMULAE (BLACKMAN 3.4)

- The formula for ionic compounds is the same as the empirical formula
- For molecules, the molecular formula and empirical are usually different
- If the experimental molecular mass is available, the empirical formula can be converted into the molecular formula
- The molecular formula will be a common multiplier times all the coefficients in the empirical formula

EXAMPLE

"A hydrocarbon was found to have the composition C = 92.3% and H = 7.7%. Find the empirical formula? Find the molecular formula, if the molar mass were: (i) 26 g mol^{-1} , or (ii) 78 g mol^{-1}."

Consider 100 g of the hydrocarbon. (do this as a matter of routine)

Weight of C in the 100g = 92.3 g = 92.3/12.00 moles C = 7.69 moles.

Weight of H in the 100g = 7.7 g = 7.7/1.008 moles H = 7.64 moles.

Mole ratio of C:H = 7.69 : 7.64 = 1 : 1.007 ≈ 1:1.

∴ Atom ratio of C:H = 1:1

∴ Empirical formula of hydrocarbon is CH (i.e. "C_1H_1").

Empirical formula mass = 12.00 + 1.008 = 13.008 g mol^{-1}.

(i) Ratio of (real molar mass)/(empirical formula mass) = 26/13.008 ≈ 2/1.

∴ Real molecular formula is C_2H_2.

(ii) Ratio of (real molar mass)/(empirical formula mass) = 78/13.008 ≈ 6/1.

∴ Real molecular formula is C_6H_6.

A compound was found to have the composition:
Na = 20.7%, H = 0.91%, P = 27.9% and O = 50.5%.
The molar mass is 222 g mol^{-1}.
Find the empirical and molecular formula.

Consider 1 mole of compound. 1 mole of compound = 222 g.

20.7% of its mass is Na,
0.91 % of its mass is H,
27.9 % of its mass is P,
50.5 % of its mass is O.

Mass Na = (0.207 x 222) g = 45.95 g ; Moles Na = (45.95) / 23 = **2**

Mass H = (0.0091 x 222) g = 2.02 g ; Moles H = (2.02) / 1.008 = **2**

Mass P = (0.279 x 222) g = 61.93 g ; Moles P = (61.93) / 31.45 = **2**

Mass O = (0.505 x 222) g = 112 g ; Moles O = (112) / 16.01 = **7**

Empirical and 'Molecular' Formula = $Na_2H_2P_2O_7$