CHEMICAL CALCULATIONS - RELATING MASS AND ATOMS

$$Na_2CO_3 + 2HCl \rightarrow H_2O + CO_2 + 2NaCl$$

Chemical equations are written and balanced in terms of ATOMS and MOLECULES

- While chemical equations are written in terms of ATOMS and MOLECULES, that's NOT how we often measure substances in lab!

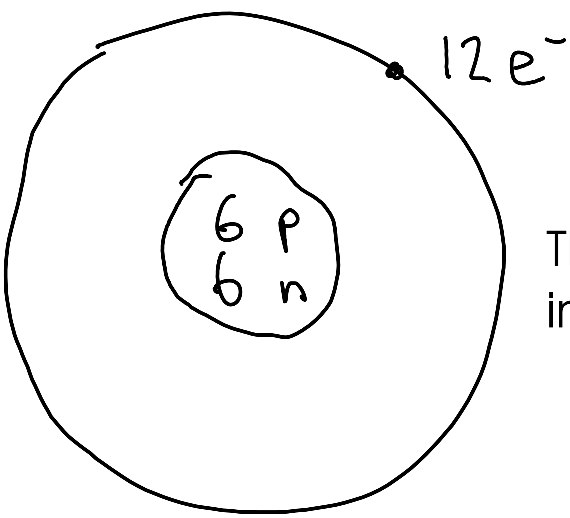
- measurements are usually MASS (and sometimes VOLUME), NOT number of atoms or molecules!

THE MOLE CONCEPT

- A "mole" of atoms is 6.022×10^{23} atoms

Why so big? Because atoms are so small!

- Why - in the metric dominated world of science - do we use such a strange number for quantity of atoms?



carbon-12

The mole is also defined as the number of carbon-12 atoms in exactly 12 g of carbon-12

THE MOLE CONCEPT

- Why define the mole based on an experimentally-measured number?

- The atomic weight of an element (if you put the number in front of the unit GRAMS) is equal to the mass of ONE MOLE of atoms of that element!

Carbon (C): Atomic mass 12.01 ~~amu~~ $\rightarrow$ $\boxed{12.01\ g}$

$\downarrow$

the mass of ONE MOLE of naturally-occurring carbon atoms

Magnesium (Mg): 24.31 g = the mass of ONE MOLE OF MAGNESIUM ATOMS

- So, using the MOLE, we can directly relate a mass and a certain number of atoms!

RELATING MASS AND MOLES

- Use DIMENSIONAL ANALYSIS (a.k.a "drag and drop")

- Need CONVERSION FACTORS - where do they come from?

- We use ATOMIC WEIGHT as a conversion factor.

Mg : 24.31 | 24.31 g Mg = 1 mol Mg

Atomic mass

"mol" is the abbreviation for "mole"

Example: How many moles of atoms are there in 250. g of magnesium metal?

Use the atomic weight of magnesium: 24.31 g Mg = 1 mol Mg

$$250.\,g\,Mg \times \frac{1\,mol\,Mg}{24.31\,g\,Mg} = \boxed{10.3\,mol\,Mg}$$

Example: You need 1.75 moles of iron. What mass of iron do you need to weigh out on the balance?

Fe: 55.85

55.85 g Fe = 1 mol Fe

$$1.75 \text{ mol Fe} \times \frac{55.85 \text{ g Fe}}{1 \text{ mol Fe}} = \boxed{97.7 \text{ g Fe}}$$

WHAT ABOUT COMPOUNDS? FORMULA WEIGHT

Example: 25.0 g of WATER contain how many MOLES of water molecules?

H_2O: H : 2 x 1.008 = 2.016

O : 1 x 16.00 = 16.00

18.016 "Formula weight" of water

Formula weight = mass of one mole of either an element OR a compound

$18.016 \text{ g } H_2O = 1 \text{ mol } H_2O$

$$25.0 \text{ g } H_2O \times \frac{1 \text{ mol } H_2O}{18.016 \text{ g } H_2O} = \boxed{1.39 \text{ mol } H_2O}$$

Formula weight goes by several names:

- For atoms, it's the same thing as ATOMIC WEIGHT
- For molecules, it;s called MOLECULAR WEIGHT
- Also called "MOLAR MASS"

Example: How many grams of ammonium carbonate do we need to weigh out to get 3.65 moles of ammonium carbonate?

Find the formula: NH_4^+ CO_3^{2-}

NH_4^+

$(NH_4)_2CO_3$

N : 2 × 14.01

H : 8 × 1.008

C : 1 × 12.01

O : 3 × 16.00

96.094

$96.094\ g\ (NH_4)_2CO_3 = 1\ mol\ (NH_4)_2CO_3$

$$3.65\ mol\ (NH_4)_2CO_3 \times \frac{96.094\ g\ (NH_4)_2CO_3}{1\ mol\ (NH_4)_2CO_3} = \boxed{351\ g\ (NH_4)_2CO_3}$$

PERCENTAGE COMPOSITION

- sometimes called "percent composition" or "percent composition by mass"
- the percentage of each element in a compound, expressed in terms of mass

Example: Find the percentage composition of ammonium nitrate.

NH_4NO_3 : N : $2 \times 14.01 = 28.02$

H : $4 \times 1.008 = 4.032$

O : $3 \times 16.00 = 48.00$

$80.052\ g\ NH_4NO_3 = 1\ mol\ NH_4NO_3$

These numbers are the masses of each element in a mole of the compound!

$$\%N : \frac{28.02\ g}{80.052\ g} \times 100\% = 35.00\%\ N$$

$$\%H : \frac{4.032\ g}{80.052\ g} \times 100\% = 5.04\%\ H$$

$$\%O : \frac{48.00\ g}{80.052\ g} \times 100\% = 59.96\%\ O$$

100.00%

So far, we have

- looked at how to determine the composition by mass of a compound from a formula
- converted from MASS to MOLES (related to the number of atoms/molecules)
- converted from MOLES to MASS

Are we missing anything?

- What about SOLUTIONS, where the desired chemical is not PURE, but found DISSOLVED IN WATER?
- How do we deal with finding the moles of a desired chemical when it's in solution?

MOLAR CONCENTRATION *

- unit: MOLARITY (M): moles of dissolved substance per LITER of solution

$$M = \text{molarity} = \frac{\text{moles of SOLUTE}}{\text{L SOLUTION}}$$

6.0 $\underline{M}$ HCl solution: $\frac{6.0 \text{ mol HCl}}{\text{L}}$

If you have 0.250 L (250 mL) of 6.0 M HCl, how many moles of HCl do you have?

6.0 mol HCl = L solution

$$0.250 \text{ L solution} \times \frac{6.0 \text{ mol HCl}}{\text{L solution}} = \boxed{1.50 \text{ mol HCl}}$$

*See SECTIONS 4.7 - 4.10 for more information about MOLARITY and solution calculations (p 154 - 162)

If you need 0.657 moles of hydrochloric acid, how many liters of 0.0555 M HCl do you need to measure out?

0.0555 mol HCl = L

$$0.657 \text{ mol HCl} \times \frac{\text{L}}{0.0555 \text{ mol HCl}} = \boxed{11.8 \text{ L}}$$

11,800 mL

This is a bit large for measuring in lab glassware, so we should probably find a more concentrated solution!

What if we used 6.00 M HCl?

6.00 mol HCl = L

$$0.657 \text{ mol HCl} \times \frac{\text{L}}{6.00 \text{ mol HCl}} = \boxed{0.110 \text{ L}}$$

$11\bar{0}$ mL

Use a 250 mL graduated cylinder, or do 2 measurements in a 100 mL cylinder.

CHEMICAL CALCULATIONS CONTINUED: REACTIONS

- Chemical reactions proceed on an ATOMIC basis, NOT a mass basis!

- To calculate with chemical reactions (i.e. use chemical equations), we need everything in terms of ATOMS ... which means MOLES of atoms

$$2\,Al(s) + 3\,Br_2(l) \longrightarrow 2\,AlBr_3(s)$$

coefficients are in terms of atoms and molecules!

2 atoms Al = 3 molecules Br_2 = 2 formula units $AlBr_3$

2 mol Al = 3 mol Br_2 = 2 mol $AlBr_3$

- To do chemical calculations, we need to:
  - Relate the amount of substance we know (mass or volume) to a number of moles
  - Relate the moles of one substance to the moles of another using the equation
  - Convert the moles of the new substance to mass or volume as desired

$$2\,Al(s) + 3\,Br_2(l) \longrightarrow 2\,AlBr_3(s)$$

* Given that we have 25.0 g of liquid bromine, how many grams of aluminum would we need to react away all of the bromine? How many grams of aluminum bromide would be produced?

1. Convert grams of bromine to moles: Need formula weight Br_2: $2 \times 79.90 = 159.80$

$$159.80\,g\,Br_2 = 1\,mol\,Br_2$$

$$25.0\,g\,Br_2 \times \frac{1\,mol\,Br_2}{159.80\,g\,Br_2} = 0.15645\,mol\,Br_2$$

2. Use the chemical equation to relate moles of bromine to moles of aluminum

$$2\,mol\,Al = 3\,mol\,Br_2$$

$$0.15645\,mol\,Br_2 \times \frac{2\,mol\,Al}{3\,mol\,Br_2} = 0.10430\,mol\,Al$$

3. Convert moles aluminum to mass: Need formula weight Al: 26.98

$$26.98\,g\,Al = 1\,mol\,Al$$

$$0.10430\,mol\,Al \times \frac{26.98\,g\,Al}{1\,mol\,Al} = \boxed{2.81\,g\,Al}$$

Aluminum bromide: Use conservation of mass!

25.0 g + 2.81 g = 27.8 g

You can combine all three steps on one line if you like!

$$25.0\,g\,Br_2 \times \frac{1\,mol\,Br_2}{159.80\,g\,Br_2} \times \frac{2\,mol\,Al}{3\,mol\,Br_2} \times \frac{26.98\,g\,Al}{1\,mol\,Al} = \boxed{2.81\,g\,Al}$$

1 2 3

You can solve the second part of the question using CONSERVATION OF MASS - since there's only a single product and you already know the mass of all reactants.

$$\begin{array}{r} 25.0\,g\,Br_2 \\ +\ 2.81\,g\,Al \\ \hline 27.8\,g\,AlBr_3 \end{array}$$

But ...

...what would you have done to calculate the mass of aluminum bromide IF you had NOT been asked to calculate the mass of aluminum FIRST?

$$25.0\,g\,Br_2 \times \frac{1\,mol\,Br_2}{159.80\,g\,Br_2} \times \frac{2\,mol\,AlBr_3}{3\,mol\,Br_2} \times \frac{266.694\,g\,AlBr_3}{1\,mol\,AlBr_3} = 27.8\,g$$

1 convert mass bromine to moles

2 convert moles bromine to moles aluminum bromide

3 convert moles aluminum bromide to mass

Example:

How many milliliters of 6.00M hydrochloric acid is needed to completely react with 25.0 g of sodium carbonate?

$$2HCl(aq) + Na_2CO_3(s) \longrightarrow H_2O(l) + CO_2(g) + 2NaCl(aq)$$

1 - Convert mass of sodium carbonate to moles using formula weight

2 - Convert moles of sodium carbonate to moles hydrochloric acid using chemical equation

3 - Convert moles of hydrochloric acid to volume using concentration (M = moles/L)

- Convert mass of sodium carbonate to moles using formula weight

Na_2CO_3: Na : 2×22.99

C : 1×12.01

O : 3×16.00

105.99

$105.99\,g\ Na_2CO_3 = 1\ mol\ Na_2CO_3$

$$25.0\,g\ Na_2CO_3 \times \frac{1\ mol\ Na_2CO_3}{105.99\,g\ Na_2CO_3} = 0.235871\ mol\ Na_2CO_3$$

Example:

How many milliliters of 6.00M hydrochloric acid is needed to completely react with 25.0 g of sodium carbonate?

$$2HCl(aq) + Na_2CO_3(s) \longrightarrow H_2O(l) + CO_2(g) + 2NaCl(aq)$$

- Convert moles of sodium carbonate to moles hydrochloric acid using chemical equation

$$2 \text{ mol } HCl = 1 \text{ mol } Na_2CO_3$$

$$0.235871 \text{ mol } Na_2CO_3 \times \frac{2 \text{ mol } HCl}{1 \text{ mol } Na_2CO_3} = 0.471743 \text{ mol } HCl$$

- Convert moles of hydrochloric acid to volume using concentration (M = moles/L)

$$6.00 \text{ mol } HCl = L \qquad mL = 10^{-3} L$$

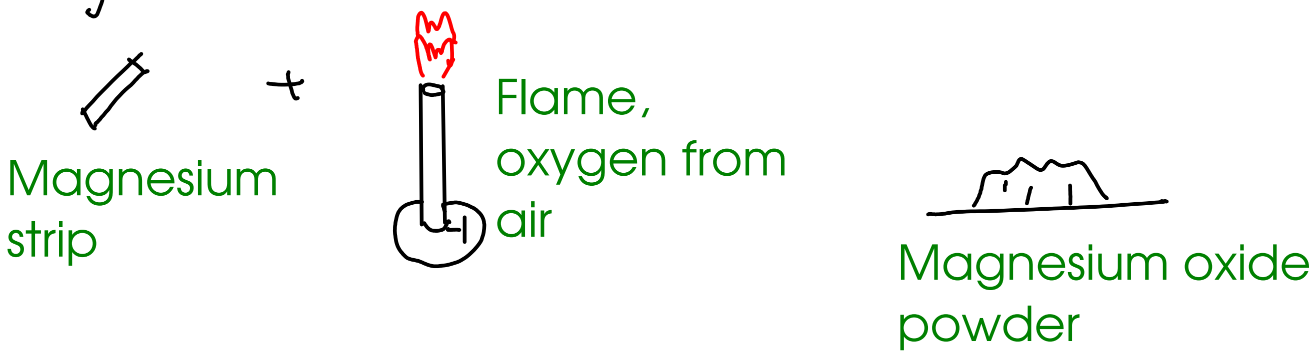
$$0.471743 \text{ mol } HCl \times \frac{L}{6.00 \text{ mol } HCl} \times \frac{mL}{10^{-3} L} = \boxed{78.6 \text{ mL}}$$

This last step converts L to mL because the problem statement specifically asked for mL.

CONCEPT OF LIMITING REACTANT

- When does a chemical reaction STOP?

$$2\,Mg(s) + O_2(g) \xrightarrow{\Delta} 2\,MgO(s)$$



- When does this reaction stop? When burned in open air, this reaction stops when all the MAGNESIUM STRIP is gone. We say that the magnesium is LIMITING.

- This reaction is controlled by the amount of available magnesium

- At the end of a chemical reaction, the LIMITING REACTANT will be completely consumed, but there may be amount of OTHER reactants remaining. We do chemical calculations in part to minimize these "leftovers".

These are often called "excess" reactants, or reactants present "in excess"