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!

Na_2CO_3 solid

HCl solution

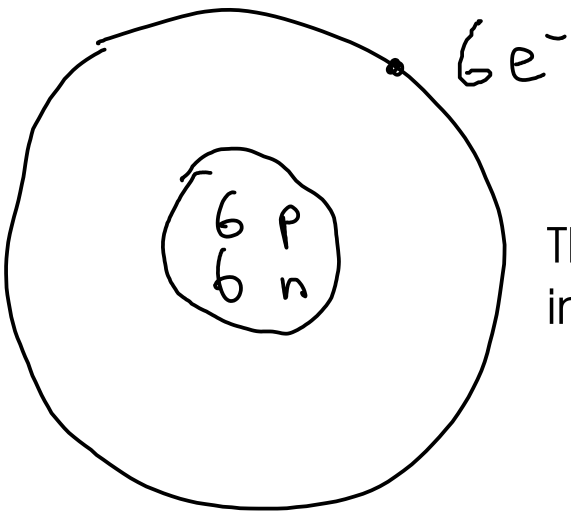
... so how do we relate atoms and molecules with things we routinely measure in lab - like grams and milliliters?

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~~ → $\boxed{12.01\ g}$

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.

$$Mg : 24.31 \quad \Big| \quad 24.31\ g\ Mg = 1\ mol\ Mg$$

"mol" is the abbreviation for "mole"

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

$$24.31\ g\ Mg = mol\ Mg$$

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

Note: Atomic weights are measured numbers, so they DO have significant figures.

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

$$55.85\ g\ Fe = mol\ Fe$$

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

WHAT ABOUT COMPOUNDS? FORMULA WEIGHT

Example: 25.0 g of WATER contain how many MOLES of water molecules?
(H_2O)

H_2O

$$H: 2 \times 1.008 = 2.016$$
$$O: 1 \times 16.00 = 16.00$$
$$18.016$$

FORMULA WEIGHT of water

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

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

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

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?

First, find the CHEMICAL FORMULA of ammonium carbonate!

$NH_4^+ \quad CO_3^{2-}$

$(NH_4)_2CO_3$

Next, find the FORMULA WEIGHT of ammonium carbonate:

N : 2 x 14.01

H : 8 x 1.008

C : 1 x 12.01

O : 3 x 16.00

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

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

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_4^+ NO_3^-

$\underline{NH_4NO_3}$:

N : 2 x 14.01 = 28.02

H : 4 x 1.008 = 4.032

O : 3 x 16.00 = 48.00

80.052 g NH_4NO_3 = mol NH_4NO_3

%N : $\frac{28.02 \text{ g N}}{80.052 \text{ g total}}$ x 100% = 35.00 % N

%H : $\frac{4.032 \text{ g H}}{80.052 \text{ g total}}$ x 100% = 5.04 % H

%O : $\frac{48.00 \text{ g O}}{80.052 \text{ g total}}$ x 100% = 59.96 % O

These percentages should sum to approximately 100%, but there may be a little bit of roundoff error depending on which decimal place you round to!

A few more examples...

Use FORMULA WEIGHT when relating mass and moles

You have a 250.g bottle of silver(I) chloride (AgCl). How many moles of AgCl do you have?

AgCl: Ag: 1 x 107.9

Cl: 1 x 35.45

143.35 g AgCl = mol AgCl

$$250.\text{ g AgCl} \times \frac{\text{mol AgCl}}{143.35\text{ g AgCl}} = \boxed{1.74\text{ mol AgCl}}$$

How many grams of NaOH are present in a 1.50 mole sample of NaOH?

NaOH: Na: 1 x 22.99

O: 1 x 16.00

H: 1 x 1.008

= mol NaOH

$$1.50\text{ mol NaOH} \times \frac{39.998\text{ g NaOH}}{\text{mol NaOH}} = \boxed{60.0\text{ g NaOH}}$$

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

$$\underline{2}Al(s) + \underline{3}Br_2(l) \longrightarrow \underline{2}AlBr_3(s)$$

coefficients are in terms of atoms and molecules!

$$\boxed{2 \text{ atoms } Al = 3 \text{ molecules } Br_2 = 2 \text{ formula units } AlBr_3}$$

$$\boxed{2 \text{ mol } Al = 3 \text{ mol } Br_2 = 2 \text{ mol } AlBr_3}$$ *

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