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!

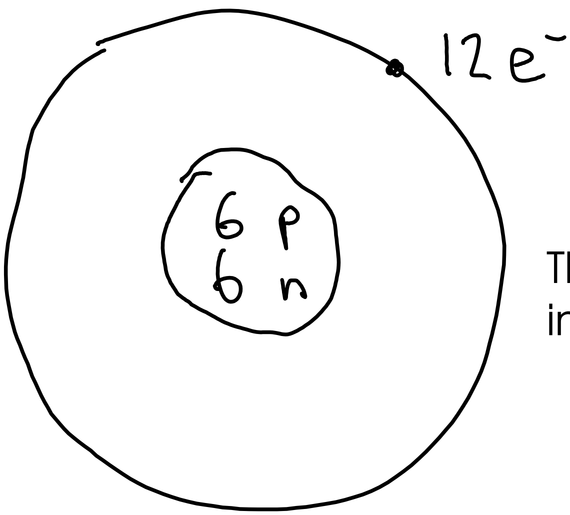
- measurements are usually MASS (and sometimes VOLUME), NOT number of atoms or molecules!

THE MOLE CONCEPT

- A "mole" of atoms is 6.022 $\times 10^{23}$ 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~~ → $\boxed{12.01\ \text{g}}$

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 | 24.31 g Mg = mol Mg

Atomic mass

"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

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

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

$$55.85\ g\ Fe = mol\ Fe$$ (from periodic table)

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

WHAT ABOUT COMPOUNDS? FORMULA WEIGHT

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

H_2O: H : 2 x 1.008 = 2.016

O : 1 x 16.00 = 16.00

18.016 ← FORMULA WEIGHT of water

FORMULA WEIGHT is the mass of one mole of either an element OR a compound.

18.016 g H_2O = 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 barium chloride do we need to weigh out to get 3.65 moles of barium chloride?

First, find the formula of the compound!

Ba^{2+} Cl^-

Cl^-

$BaCl_2$

Second, find the FORMULA WEIGHT

Ba : 1 x 137.3

Cl : 2 x 35.45

208.2 g $BaCl_2$ = mol $BaCl_2$

Finally, calculate the mass ...

$$3.65 \text{ mol } BaCl_2 \times \frac{208.2 \text{ g } BaCl_2}{\text{mol } BaCl_2} = \boxed{76\bar{0} \text{ g } BaCl_2}$$

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 barium chloride.

$BaCl_2$: Ba : $1 \times 137.3 = \boxed{137.3}$

Cl : $2 \times 35.45 = \boxed{70.90}$

208.2 g $BaCl_2$ = mol $BaCl_2$

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

Ba: $\frac{137.3\text{ g Ba}}{208.2\text{ g BaCl}_2} \times 100 = \boxed{65.95\%\text{ Ba}}$

Cl: $\frac{70.90\text{ g Cl}}{208.2\text{ g BaCl}_2} \times 100 = \boxed{34.05\%\text{ Cl}}$

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

dissolved substance

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

6.0 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

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

*See SECTIONS 4.7 - 4.10 for more information about MOLARITY and solution calculations (p 154 - 162 - 9th edition) (p 156-164 - 10th edition)

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

$0.0555 \text{ mol HCl} = \text{L}$

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

11800 mL

For this particular situation, we'd use the 6.00 M HCl, since it's volume would be easier to measure in the lab. We typically have a range of concentrations of common reagents in lab because we want easy to measure volumes!

What if we used 6.00 M HCl?

$6.00 \text{ mol HCl} = \text{L}$

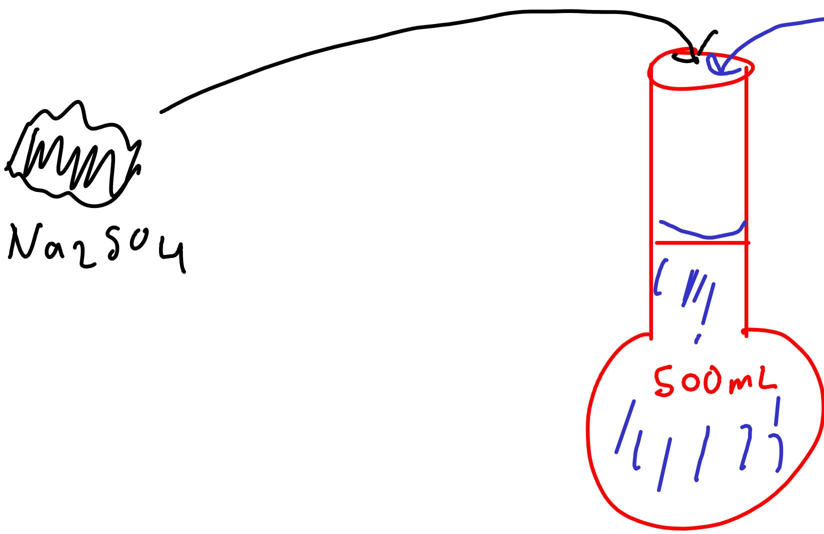
$$0.657 \text{ mol HCl} \times \frac{\text{L}}{6.00 \text{ mol HCl}} = \boxed{0.110 \text{ L}}$$

$11\bar{0}$ mL

Example: How would we prepare 500. mL of 0.500 M sodium sulfate in water?

Na_2SO_4 : 142.05 g/mol

Dissolve the appropriate amount of sodium sulfate into enough water to make 500. mL of solution.



volumetric flask

A VOLUMETRIC FLASK is a flask that is designed to precisely contain a certain volume of liquid.

VOLUMETRIC FLASKS are used to prepare solutions.

First, we figure out the MOLES of sodium sulfate in 500 mL of 0.500 M solution. Then, we change that number of moles to mass using formula weight.

$0.500 \text{ mol } Na_2SO_4 = L \qquad mL = 10^{-3} L$

$$500.\, mL \times \frac{10^{-3} L}{mL} \times \frac{0.500 \text{ mol } Na_2SO_4}{L} = 0.250 \text{ mol } Na_2SO_4$$

$142.05\, g\ Na_2SO_4 = \text{mol } Na_2SO_4$

$$0.250 \text{ mol } Na_2SO_4 \times \frac{142.05\, g\ Na_2SO_4}{\text{mol } Na_2SO_4} = \boxed{35.5\, g\ Na_2SO_4}$$

Weigh out 35.5 grams sodium sulfate into a 500 mL volumetric flask and add water to the mark...

More on MOLARITY

To prepare a solution of a given molarity, you generally have two options:

1. Weigh out the appropriate amount of solute, then dilute to the desired volume with solvent (usually water)

"stock solution"

2. Take a previously prepared solution of known concentration and DILUTE it with solvent to form a new solution

- Use DILUTION EQUATION

The dilution equation is easy to derive with simple algebra.

$$M \times V$$

$$\frac{mol}{L} \times L = \text{moles solute}$$

... but when you dilute a solution, the number of moles of solute REMAINS CONSTANT. (After all, you're adding only SOLVENT)

$$M_1 V_1 = M_2 V_2$$

Since the number of moles of solute stays the same, this equality must be true!

before diution

after dilution

$M_1 V_1 = M_2 V_2$ ... the "DILUTION EQUATION"

M_1 = molarity of concentrated solution

V_1 = volume of concentrated solution

M_2 = molarity of dilute solution

V_2 = volume of dilute solution (total volume, not volume of added solvent!)

The volumes don't HAVE to be in liters, as long as you use the same volume UNIT for both volumes!

Example: Take the 0.500 M sodium sulfate we discussed in the previous example and dilute it to make 150. mL of 0.333 M solution. How many mL of the original solution will we need to dilute?

$M_1 V_1 = M_2 V_2$

$M_1 = 0.500\,M$ $M_2 = 0.333\,M$

$V_1 = ?$ $V_2 = 150.\,mL$

$(0.500\,M)V_1 = (0.333\,M)(150.\,mL)$

$V_1 = \boxed{99.9\,mL \text{ of } 0.500\,M\ Na_2SO_4}$

Measure out 99.9 mL of 0.500 M sodium sulfate, then add water until the total volume equals 150. mL.

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!

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

- 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?

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

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

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

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 $Al: 26.98$

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

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

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

1 $154.80\,g\ Br_2 = mol\ Br_2$ 2 $2\ mol\ Al = 3\ mol\ Br_2$ 3 $26.98\,g\ Al = mol\ Al$

$$25.0\,g\ Br_2 \times \frac{mol\ Br_2}{154.80\,g\ Br_2} \times \frac{2\ mol\ Al}{3\ mol\ Br_2} \times \frac{26.98\,g\ Al}{mol\ Al} = \boxed{2.81\,g\ Al}$$

1 2 3

Things we can do:

If we have ...	... and we need ...	Use ...
MASS	MOLES	FORMULA WEIGHT
SOLUTION VOLUME	MOLES	MOLAR CONCETRATION (MOLARITY)
MOLES OF A	MOLES OF B	BALANCED CHEMICAL EQUATION

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 25.0 grams sodium carbonate to moles. Use FORMULA WEIGHT.
2) Convert moles sodium carbonate to moles HCl. Use CHEMICAL EQUATION.
3) Convert moles HCl to volume HCl solution. Use MOLARITY (6.0 M HCl)

---

1 Na_2CO_3 – Na: 2 x 22.99
C: 1 x 12.01
O: 3 x 16.00

$105.99\ g\ Na_2CO_3 = mol\ Na_2CO_3$

$$25.0\ g\ Na_2CO_3 \times \frac{mol\ Na_2CO_3}{105.99\ g\ Na_2CO_3} = 0.2358713086\ mol\ Na_2CO_3$$

---

2 $2\ mol\ HCl = mol\ Na_2CO_3$

$$0.2358713086\ mol\ Na_2CO_3 \times \frac{2\ mol\ HCl}{mol\ Na_2CO_3} = 0.4717426172\ mol\ HCl$$