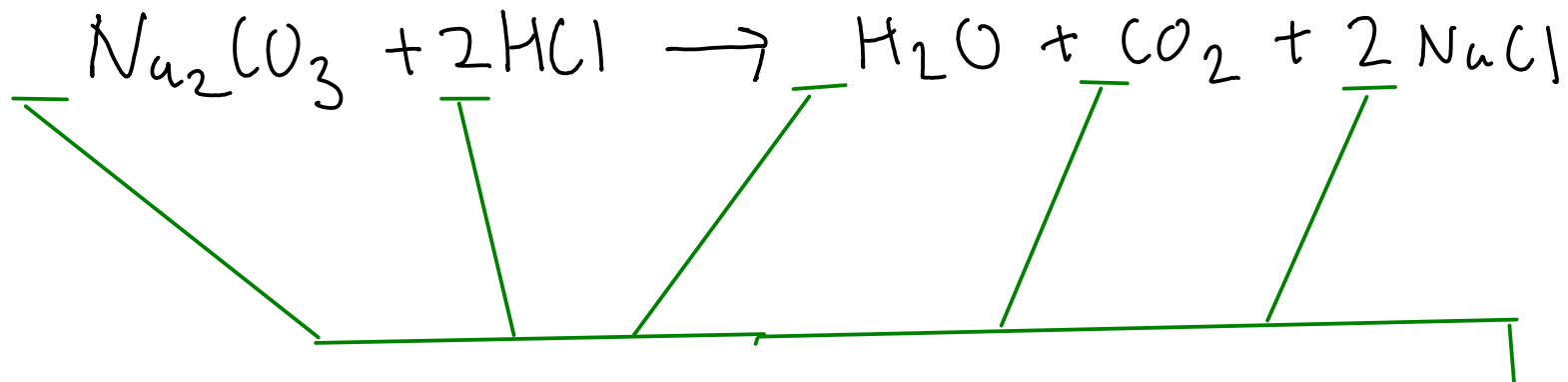


## CHEMICAL CALCULATIONS - RELATING MASS AND ATOMS



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

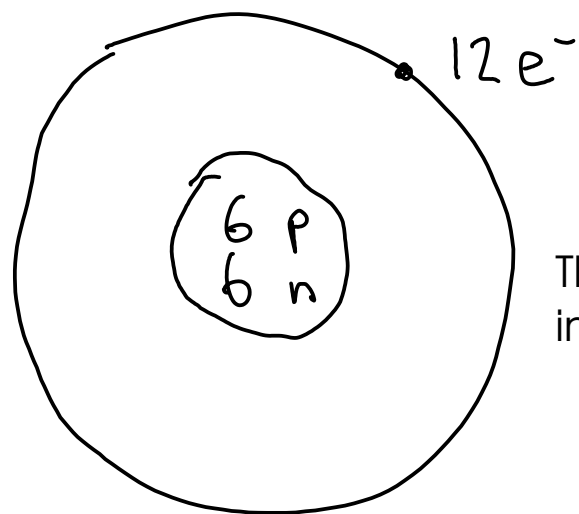
- While chemical equations are written in terms of ATOMS and MOLECULES, that's NOT how we often measure substances in lab!
- measurements are usually MASS (and sometimes VOLUME), NOT number of atoms or molecules!

## 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!

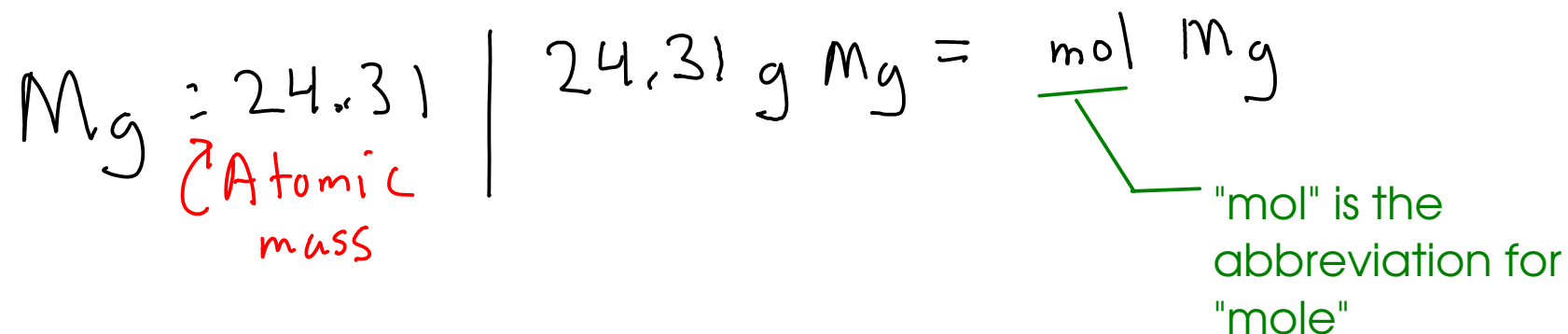
Carbon (C): Atomic mass 12.01 amu ~~amu~~ → 12.01 g  
↓  
the mass of ONE MOLE of naturally-occurring carbon atoms

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.



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

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

ATOMIC WEIGHT is a MEASURED number - in other words, it has significant figures. Usually we can find atomic weights with more significant figures if necessary.

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

Fe: 55.85g Fe = mol Fe

↪ Atomic weight  
of iron from  
periodic  
table

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

## WHAT ABOUT COMPOUNDS? FORMULA WEIGHT

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

$$\text{H}_2\text{O} : \quad \text{H} : 2 \times 1.008 = 2.016$$

$$\quad \quad \quad \text{O} : 1 \times 16.00 = 16.00$$

18.016 ← FORMULA WEIGHT of water

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

$$18.016 \text{ g H}_2\text{O} = 1 \text{ mol H}_2\text{O}$$

$$25.0 \text{ g H}_2\text{O} \times \frac{1 \text{ mol H}_2\text{O}}{18.016 \text{ g H}_2\text{O}} = 1.39 \text{ mol H}_2\text{O}$$

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 FORMULA  
of  
ammonium  
carbonate!



Next, find FORMULA WEIGHT:

$$\text{N: } 2 \times 14.01$$

$$\text{H: } 8 \times 1.008$$

$$\text{C: } 1 \times 12.01$$

$$\text{O: } 3 \times 16.00$$

---


$$96.094 \text{ g } (\text{NH}_4)_2\text{CO}_3 = \text{mol } (\text{NH}_4)_2\text{CO}_3$$

$$3.65 \text{ mol } (\text{NH}_4)_2\text{CO}_3 \times \frac{96.094 \text{ g } (\text{NH}_4)_2\text{CO}_3}{\text{mol } (\text{NH}_4)_2\text{CO}_3} = 351 \text{ g } (\text{NH}_4)_2\text{CO}_3$$

## 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.

$$\text{NH}_4\text{NO}_3 : \text{N} : 2 \times 14.01 = 28.02$$

$$\text{H} : 4 \times 1.008 = 4.032$$

$$\text{O} : 3 \times 16.00 = 48.00$$

$$\underline{80.052 \text{ g NH}_4\text{NO}_3 = \text{mol NH}_4\text{NO}_3}$$

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

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

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

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

Check ... should all sum to 100% ... within roundoff error.



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

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

↙ dissolved substance

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

If you have 0.250 L (250 mL) of 6.0 M HCl, how many moles of HCl do you have?  $6.0 \text{ mol HCl} = \text{L}$

$$0.250 \text{ L} \times \frac{6.0 \text{ mol HCl}}{\text{L}} = 1.5 \text{ mol HCl}$$

\*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

This volume is much too large for typical lab-scale work. We should use a more concentrated solution to get 0.657 mol HCl!

What if we used 6.00 M HCl?

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

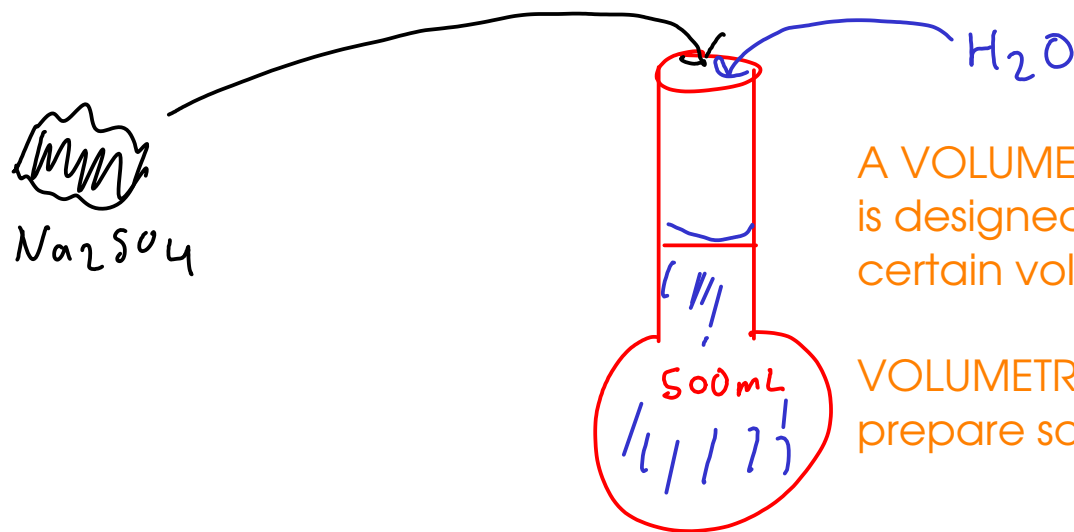
$$0.657 \text{ mol HCl} \times \frac{\text{L}}{6.00 \text{ mol HCl}} = \boxed{0.110 \text{ L}}$$

110 mL

This is a more reasonable volume for lab-scale work.

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

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



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

VOLUMETRIC FLASKS are used to prepare solutions.

volumetric flask

We know we need 500. mL solution, and we know that it must be 0.500 M sodium sulfate. From that, we calculate the moles sodium sulfate we need. Then convert the moles sodium sulfate to mass using formula weight.

$$0.500 \text{ mol Na}_2\text{SO}_4 = \text{L} \quad | \quad \text{mL} = 10^{-3} \text{ L} \quad | \quad 142.05 \text{ g Na}_2\text{SO}_4 = \text{mol Na}_2\text{SO}_4$$

$$500 \text{ mL} \times \frac{10^{-3} \text{ L}}{\text{mL}} \times \frac{0.500 \text{ mol Na}_2\text{SO}_4}{\text{L}} \times \frac{142.05 \text{ g Na}_2\text{SO}_4}{\text{mol Na}_2\text{SO}_4} = \boxed{35.5 \text{ g Na}_2\text{SO}_4}$$

To prepare the solution, we weigh 35.5 grams of sodium sulfate into a 500. mL volumetric flask, then dilute to the mark with distilled water.

## 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)

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

"stock solution"

- Use DILUTION EQUATION

The dilution equation is easy to derive with simple algebra.

$$M \times V$$

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

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

$$M_1 V_1 = M_2 V_2$$

before  
dilution

after  
dilution

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

$$M_1 V_1 = M_2 V_2 \quad \dots \text{the "DILUTION EQUATION"}$$

$M_1$  = 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?

$$M_1 V_1 = M_2 V_2 \quad M_1 = 0.500 \text{ M} \quad M_2 = 0.333 \text{ M}$$

$$V_1 = ??? \quad V_2 = 150. \text{ mL}$$

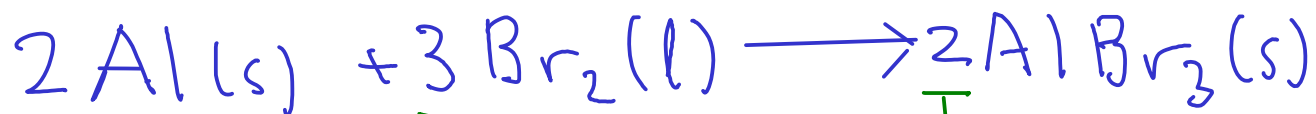
$$(0.500 \text{ M}) V_1 = (0.333 \text{ M}) (150. \text{ mL})$$

$$V_1 = 99.9 \text{ mL of } 0.500 \text{ M Na}_2\text{SO}_4$$

Take 99.9 mL of 0.500 M sodium sulfate, and dilute with enough water to make 150. mL of solution. (Ideally, use 150 mL volumetric, otherwise add 50.1 mL water)

## CHEMICAL CALCULATIONS CONTINUED: REACTIONS

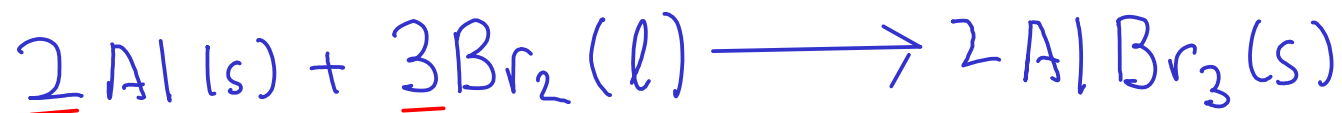
- Chemical reactions proceed on an ATOMIC basis, NOT a mass basis!
- To calculate with chemical reactions (i.e. use chemical equations), we need everything in terms of ATOMS ... which means MOLES of atoms



coefficients are in terms of atoms and molecules!



- 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



\* 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  $\text{Br}_2$ :  $\frac{2 \times 79.90}{159.80}$

$$159.80 \text{ g Br}_2 = 1 \text{ mol Br}_2$$

$$25.0 \text{ g Br}_2 \times \frac{1 \text{ mol Br}_2}{159.80 \text{ g Br}_2} = 0.15645 \text{ mol Br}_2$$

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

$$2 \text{ mol Al} = 3 \text{ mol Br}_2$$

$$0.15645 \text{ mol Br}_2 \times \frac{2 \text{ mol Al}}{3 \text{ mol Br}_2} = 0.10430 \text{ mol Al}$$

③ Convert moles aluminum to mass: Need formula weight  $\text{Al}$ : 26.98

$$26.98 \text{ g Al} = 1 \text{ mol Al}$$

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



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

$$25.0 \text{ g Br}_2 \times \frac{1 \text{ mol Br}_2}{159.80 \text{ g Br}_2} \times \frac{2 \text{ mol Al}}{3 \text{ mol Br}_2} \times \frac{26.98 \text{ g Al}}{1 \text{ mol Al}} = 2.81 \text{ g Al}$$

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.

$$\begin{array}{r} 25.0 \text{ g Br}_2 \\ + 2.81 \text{ g Al} \\ \hline 27.8 \text{ g AlBr}_3 \end{array}$$

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?

$$25.0 \text{ g Br}_2 \times \frac{1 \text{ mol Br}_2}{159.80 \text{ g Br}_2} \times \frac{2 \text{ mol AlBr}_3}{3 \text{ mol Br}_2} \times \frac{266.694 \text{ g AlBr}_3}{1 \text{ mol AlBr}_3} = 27.8 \text{ g AlBr}_3$$

①
②
③

convert mass  
bromine  
to moles

convert moles  
bromine to  
moles aluminum  
bromide

convert moles  
aluminum  
bromide  
to mass