Chemical Quantities: Stoichiometry and the Mole

This is trying to summarize what we have learned up to this point: formulas, names, conversions, moles, quantities, reaction types, balancing equations, etc., and to show how they come together. Every little part is important. Every part contributes to the whole of chemistry.

A number of the parts can be broken down into simple steps, although there may be steps-within-steps. If you follow the steps you can get to the answer. Think about the "steps" I mentioned when we talked about problem solving. When we learned how to write the names of compounds for their formulas, and the formulas for the names. When we do conversions and stoichiometry. I am half cliche when I describe this process as "following the yellow brick road."

In chemistry most things are ALWAYS done the same way. The particular application may be different, but the process is the same.

Counting by weighing

- Why use moles?
  - Many properties depend upon the number of atoms, formula units or molecules in the sample, not on the mass of the sample.
    Problem: How can the number of molecules in the sample be measured?
  - Solution: Convert sample mass to atomic mass units to molecules , using the atomic, formula or molecular mass.
  - Now you can count the number of atoms, formula units or molecules just by weighing the sample.
  - Problem: Atomic mass units are very small, and inconvenient; can we convert grams to atoms, formula units or molecules without using them?
  - Solution: Define a new unit, the **Mole** (SI unit for the **amount of substance**).
  - The mole is a unit of quantity although it is not something *by itself* that we can see, touch, or measure; and it is the ultimate factor that chemists use in talking about any substance.

- Defining moles
  - **1 mole of atoms** has a mass equal to the atomic mass in grams
    1 mole of formula units has a mass equal to the formula mass in grams
    1 mole of molecules has a mass equal to the molecular mass in grams
  - Examples:
    - 1 mole of Cu is the number of atoms in 63.55 g Cu (aka: gram atomic mass)
    - 1 mole of H_2 is the number of molecules in 2.016 g H_2 (aka: gram molecular mass)
    - 1 mole of NaCl is the number of formula units in 58.45 g NaCl (aka: gram formula mass)
    - 1 mole of $C_6H_{12}O_6$ is the number of molecules in 180.16 g $C_6H_{12}O_6$
  - **Molar Mass** is the mass of one mole of a substance. This is a more general expression than atomic mass, molecular mass or formula mass. Some people just call all of this "molecular mass"

and older literature may mention "molecular weight."

- **Avogadro's Number** is the number of atoms, formula units or molecules in one mole of a substance
- 1 mole of representative particles is 6.022×10^{23} particles *for any substance*
- 1 mole of any gas at STP (*S*tandard *T*emperature and *P*ressure: 0°C and 1 atmosphere pressure) occupies a volume of exactly 22.4 L.

Using Chemical Formulas

- chemical formulas give atom-to-atom and mole-to-mole ratios
  - Example: molecular formula $C_6H_{12}O_6$

atom-to-atom ratios	**atom-to-molecule ratios**	**mole-to-mole ratios (elements)**	**mol-to-mole ratios (compounds)**
$\frac{\text{6 atoms C}}{\text{12 atoms H}}$	$\frac{\text{6 atoms C}}{\text{1 molecule}}$	$\frac{\text{6 mole C}}{\text{12 mole H}}$	$\frac{\text{6 mole C}}{\text{1 mole } C_6H_{12}O_6}$
$\frac{\text{6 atoms C}}{\text{6 atoms O}}$	$\frac{\text{12 atoms H}}{\text{1 molecule}}$	$\frac{\text{6 mole C}}{\text{6 mole O}}$	$\frac{\text{12 mole H}}{\text{1 mole } C_6H_{12}O_6}$
$\frac{\text{12 atoms H}}{\text{6 atoms O}}$	$\frac{\text{6 atoms O}}{\text{1 molecule}}$	$\frac{\text{12 mole H}}{\text{6 mole O}}$	$\frac{\text{6 mole O}}{\text{1 mole } C_6H_{12}O_6}$

- The coefficients in a balanced chemical equation tell us the relationship between the atoms, formula units and/or molecules represented (on the atomic level) but also between moles of atoms, formula units and/or molecules (on the real world level).
  - Example: $Na_2CO_3 + 2\,HCl \longrightarrow 2\,NaCl + CO_2 + H_2O$
    - 1 formula unit of Na_2CO_3 reacts with 2 formula units of HCl to give 2 formula units of NaCl, 1 molecule of CO_2 and 1 molecule of H_2O AND
    - 1 mole of Na_2CO_3 reacts with 2 moles of HCl to give 2 moles of NaCl, 1 mole of CO_2 and 1 mole of H_2O
  - However, remember that the coefficients **do not** mean that 1 gram of Na_2CO_3 reacts with 2 grams of HCl to give 2 grams of NaCl, 1 gram of CO_2 and 1 gram of H_2O

- Problems that ask you to relate one substance to another require mole-to-mole ratios
  - Examples:
    - How many grams of H_2 can be obtained from the electrolysis of 10.0 g H_2O?
    - How many grams of CuO can be made from a piece of copper wire with a mass of 0.2134 g?
    - 2.04 g of carbon react with 5.44 g of O_2 to form 7.48 g of a compound. How many atoms of O per atom of C are in the compound?

Chemical formulas and chemical composition

- Atomic, ionic and molecular formulas tell you exactly what atoms are present in the substance and how many of each there are: Ag, O_2, Na_2CO_3 and CO_2
- Sometimes chemists expand the simple formulas in order to help describe something more about the structure: C_3H_8O vs C_3H_7OH vs CH_3-CH_2-CH_2-O-H
- **mass percent:** percent of the total sample mass contributed by a particular component
  - determine experimentally by decomposing the sample into its components and getting the mass of the separate components
    - determining water of hydration
    - combustion analysis of hydrocarbons
    - the percentage amount of any one component

- You can use an empirical formula and the mass percent to determine the molecular formula of a compound. Remember that the molecular formula is merely a whole number "multiple" of the empirical formula.

Putting It All Together: Applications and practice problems

A chemical equations shows the reactants (left side) and the products (right side) involved in a chemical reaction. A balanced equation shows, in terms of moles in the practical sense, how much of each substance is involved in the reaction. Stoichiometry is the study of the relationships of quantities of substances in a chemical reaction.

Consider the reaction:

$$FeCl_3\ (aq) + 3\ NaOH\ (aq) \longrightarrow Fe(OH)_3\ (s) + 3\ NaCl\ (aq)$$

Like in the earlier example, this balanced equation tells us: one mole of iron(III) chloride reacts with three moles of sodium hydroxide to produce one mole of iron(III) hydroxide and three moles of sodium chloride. Several mole ratio fractions are possible:

$$\frac{3\ \text{mol NaOH}}{1\ \text{mol FeCl}_3} \quad \text{or} \quad \frac{1\ \text{mol FeCl}_3}{1\ \text{mol Fe(OH)}_3} \quad \text{or} \quad \frac{3\ \text{mol NaCl}}{1\ \text{mol FeCl}_3} \quad \text{and others}$$

By this time you should recognize these as conversion factors. The first relates moles of the two reactants; the second and third relate one of the reactants to one of the products.

No matter how much of each reactant there is to start with (it is not a perfect world where we always have or need to use just the moles in the balanced equation) they will react only in the ratio of 1 mol $FeCl_3$ / 3 mol NaOH. If exactly 1 mole of $FeCl_3$ and 3 moles of NaOH are brought together, both reactants will be completely consumed. If one mole of $FeCl_3$ and five moles of NaOH are brought together, only three moles of the NaOH will react; two moles of NaOH will be left unreacted. If three moles of $FeCl_3$ and three moles of NaOH are brought together, two moles of $FeCl_3$ will remain unreacted.

EXAMPLE: What mass of sodium hydroxide is needed to react completely with 10.0 g of iron(III) chloride?

The conversion sequence is:

$$\text{g } FeCl_3 \xrightarrow{A} \text{mol } FeCl_3 \xrightarrow{B} \text{mol NaOH} \xrightarrow{C} \text{g NaOH}$$

(A) Mass to moles:

$$10.0\ \cancel{\text{g } FeCl_3} \times \frac{1 \text{ mol } FeCl_3}{162.3\ \cancel{\text{g } FeCl_3}} = 0.0616 \text{ mol } FeCl_3$$

(B) Moles to moles (using the mole ratio from the balanced chemical equation):

$$0.0616\ \cancel{\text{mol } FeCl_3} \times \frac{3 \text{ mol NaOH}}{1\ \cancel{\text{mol } FeCl_3}} = 0.185 \text{ mol NaOH}$$

(C) Moles to mass:

$$0.185\ \cancel{\text{mol NaOH}} \times \frac{40.0 \text{ g NaOH}}{1\ \cancel{\text{mol NaOH}}} = 7.40 \text{ g NaOH}$$

Steps (A), (B), and (C) may be combined:

$$10.0\ \cancel{\text{g } FeCl_3} \times \frac{1\ \cancel{\text{mol } FeCl_3}}{162.3\ \cancel{\text{g } FeCl_3}} \times \frac{3\ \cancel{\text{mol NaOH}}}{1\ \cancel{\text{mol } FeCl_3}} \times \frac{40.0 \text{ g NaOH}}{1\ \cancel{\text{mol NaOH}}} = 7.39 \text{ g NaOH}$$

==> Can you see why the answer is different when all three steps are combined? <==

EXAMPLE: What mass of iron(III) hydroxide will be formed from 10.0 g of iron(III) chloride?

The conversion sequence is:

$$\text{g } FeCl_3 \longrightarrow \text{mol } FeCl_3 \longrightarrow \text{mol } Fe(OH)_3 \longrightarrow \text{g } Fe(OH)_3$$

Combining the three steps:

$$10.0\ \cancel{\text{g } FeCl_3} \times \frac{1\ \cancel{\text{mol } FeCl_3}}{162.3\ \cancel{\text{g } FeCl_3}} \times \frac{3\ \cancel{\text{mol } Fe(OH)_3}}{1\ \cancel{\text{mol } FeCl_3}} \times \frac{106.8 \text{ g } Fe(OH)_3}{1 \text{ mol } \cancel{Fe(OH)_3}} = 6.58 \text{ g } Fe(OH)_3$$

A variation of this kind of problem is one in which you are given amounts of both reactants and asked to find the amount of product formed. Usually the amount of one of the reactants given is in excess and the yield of product is determined by the reactant present in the (stoichiometrically) smaller amount: **the limiting reactant or reagent.** One way to do this is to first decide which is the limiting reactant and then calculate the amount of product formed from that.

<u>EXAMPLE</u>: With reference to the iron(III) chloride and sodium hydroxide reaction: What mass of iron(III) hydroxide will be formed if a solution containing 10.0 g $FeCl_3$ is mixed with a solution containing 10.0 g sodium hydroxide?

You recognize this as a limiting reactant problem because masses of both reactants are given. As we discussed, one way is to find the moles of each reactant:

(D) $$10.0\ \cancel{\text{g FeCl}_3} \times \frac{1\text{ mol FeCl}_3}{162.3\ \cancel{\text{g FeCl}_3}} = 0.016\text{ mol FeCl}_3\text{ given}$$

(E) $$10.0\ \cancel{\text{g NaOH}} \times \frac{1\text{ mol NaOH}}{40.0\ \cancel{\text{g NaOH}}} = 0.250\text{ mol NaOH given}$$

Take either of these moles of reactants and calculate how much of the other reactant would be needed to react completely with it. Let us take mol $FeCl_3$:

(F) $$0.0616\ \cancel{\text{mol FeCl}_3} \times \frac{3\text{ mol NaOH}}{1\ \cancel{\text{mol FeCl}_3}} = 0.185\text{ mol NaOH needed}$$

Compare the moles of NaOH (F) with the given moles from (E), above. We see that more NaOH is available than needed. Therefore NaOH is in excess over what is needed to react with the given amount of $FeCl_3$, and the $FeCl_3$ is the limiting reactant.

To arrive at this conclusion we arbitrarily picked $FeCl_3$ to make the comparison. Suppose, instead, we would choose NaOH for the comparison. Find out how much $FeCl_3$ would be needed to completely react with the given amount of NaOH:

(G) $$0.250\ \cancel{\text{mol NaOH}} \times \frac{1\text{ mol FeCl}_3}{3\ \cancel{\text{mol NaOH}}} = 0.0833\text{ mol FeCl}_3\text{ needed}$$

Comparing this amount needed with the given amoun in (D), above, we see that less $FeCl_3$ is available than is needed. Thus, there is not enough $FeCl_3$ to react with all the available NaOH and the NaOH is in excess; the $FeCl_3$ is the limiting reactant.

Once we have determined the limiting reactant, the amount of product is calculated from the moles of the limiting reactant:

$$0.0616\ \cancel{\text{mol FeCl}_3} \times \frac{1\ \cancel{\text{mol Fe(OH)}_3}}{1\ \cancel{\text{mol FeCl}_3}} \times \frac{106.8\ \text{g Fe(OH)}_3}{1\ \cancel{\text{mol Fe(OH)}_3}} = 6.58\ \text{g Fe(OH)}_3$$

In these examples we have calculated that 6.58 g of $Fe(OH)_3$ can be obtained from 10.0 g $FeCl_3$ by our chemical reaction when $FeCl_3$ is the limiting reactant. This is the maximum amount that can be obtained from 10.0 g $FeCl_3$: this is the **theoretical yield** of $Fe(OH)_3$.

Almost always, stoichiometry calculations are theoretical yields. In actual practice this theoretical yield is very seldom realized – there are always some losses in the isolation of a reaction product, and some reactions just do not yield 100% no matter what. This means that something less than 6.48 g $Fe(OH)_3$ would be obtained from 10.0 g $FeCl_3$. This lesser amount will be some percent of the theoretical yield: it will give us the **percentage yield**.

EXAMPLE: A solution containing 10.0 g of iron(III) chloride is mixed with a solution containing an excess of sodium hydroxide. The solid iron(III) hydroxide is collected, dried, and weighed. It has a mass of 6.27 g. Calculate the percentage yield.

We have already calculated the theoretical yield several times for this reaction: 6.58 g $Fe(OH)_3$. The percentage yield is:

$$\text{Percent yield} = \frac{\text{Actual yield}}{\text{Theoretical yield}} \times 100 = \frac{6.27\ \text{g}}{6.58\ \text{g}} \times 100 = 95.3\%$$

Summary

In our discussions and in the Notes we have also looked at another way to calculate the amount of product that can be obtained in a limiting reactant problem. Either approach can be used and each has its own advantage in certain circumstances.

You should also note that, as I mentioned in my "steps" in doing stoichiometric calculations, you KNOW before you do any number crunching on your calculator whether you are heading the right way in solving the problem because the units cancel. Look back at the examples and notice the cancelled units. Do not rush ahead to using the calculator – do the preparation.

The next pages give you some practice problems.

The following balanced chemical equations will be needed for the problems that follow. You decide which equation is needed for each problem. (Challenge yourself by doing the problems without looking at these!)

(a) $2\ Al\ (s) + 3\ Cl_2\ (g) \longrightarrow 2\ AlCl_3\ (s)$

(b) $2\ Al\ (s) + 3\ H_2SO_4\ (aq) \longrightarrow Al_2(SO_4)_3\ (aq) + 3\ H_2\ (g)$

(c) $2\ Al\ (s) + 3\ ZnCl_2\ (aq) \longrightarrow 2\ AlCl_3\ (aq) + 3\ Zn\ (s)$

(d) $3\ BaCl_2\ (aq) + Al_2(SO_4)_3\ (aq) \longrightarrow 3\ BaSO_4\ (s) + 2\ AlCl_3\ (aq)$

(e) $Zn(OH)_2\ (aq) + 2\ HCl\ (aq) \longrightarrow ZnCl_2\ (aq) + 2\ H_2O\ (l)$

(f) $Ag_2SO_4\ (aq) + 2\ NaCl\ (aq) \longrightarrow 2\ AgCl\ (s) + Na_2SO_4\ (aq)$

1) What mass of barium chloride is required to react completely with 10.0 g of aluminum sulfate?

2) What mass of chlorine gas is required to react with 10.0 g of aluminum metal?

3) What mass of sodium chloride is required to react with 0.0115 mol of silver sulfate?

4) What mass of HCl, in tons, is required to react completely with 1.25 tons of zinc hydroxide?

5) How many pounds of aluminum will react with 150.0 pounds of zinc chloride?

6) What mass of silver chloride could be formed from 1.250 g of silver sulfate? What is the percent yield if 1.092 g AgCl is actually obtained?

7) What mass of barium sulfate could be formed from 155 g of aluminum sulfate? What is the percent yield if 300.15 g $BaSO_4$ is actually obtained?

8) What mass of aluminum chloride could be formed from 0.100 mol of aluminum metal? What is the percent yield if 12.5 g $AlCl_3$ is actually obtained?

9) What mass of zinc metal could be formed from 5.55 g aluminum metal reacting with an excess of zinc chloride solution? What is the percent yield if 18.93 g Zn is actually obtained?

10) What mass of aluminum sulfate, in tons, could be formed from the reaction of 1.00 ton of aluminum metal with excess sulfuric acid?

11) Reaction of hydrochloric acid with a sample of zinc hydroxide gave 0.555 g of zinc chloride. What was the mass of the zinc hydroxide sample?

12) When a barium chloride solution is mixed with a solution containing excess aluminum sulfate, 0.888 g of barium sulfate is obtained. What mass of barium sulfate was contained in the solution?

13) A 0.187 g sample of impure aluminum metaal was treated with excess sulfuric acid. 0.921 g of aluminum sulfate was obtained. Calculate the percent purity of the aluminum sample.

14) A solution containing 15.0 g of barium chloride is mixed with a solution containing 15.0 g aluminum sulfate. What mass of barium sulfate will form?

15) A solution containing 0.0252 mol of silver sulfate is mixed with a solution containing 2.52.g of sodium chloride. What mass of silver chloride will form?

16) 1.00 g of aluminum metal is treated with a solution containing 7.00 g of zinc chloride. What mass of metallic zinc will form?

17) A solution of aluminum sulfate was treated with an excess of barium chloride solution. It was determined that 5.05 g of barium sulfate and 1.93 g of aluminum chloride were formed in the reaction. What mass of aluminum sulfate was in the original solution?

18) A 0.5273 g sample of impure silver sulfate was treated with an excess sodium chloride solution. 0.3572 g of silver chloride was obtained. Calculate the percent purity of the silver sulfate sample.

19) 1.52 g of aluminum reacted with excess chlorine gas to give an 83.5% yield of aluminum chloride. Calculate this mass of aluminum chloride.

20) 2.350 g of a 72.5% pure sample of aluminum sulfate was treated with excess barium chloride solution. What mass of barium sulfate was formed?

<u>Answers to Problems</u>

1) 18.3 g $BaCl_2$
2) 39.4 g Cl_2
3) 1.35 g NaCl
4) 0.918 ton HCl
5) 19.78 lbs Al
6) 1.149 g AgCl; 95.04% pure
7) 317 g $BaSO_4$; 94.7%
8) 13.4 g $AlCl_3$; 93.3%
9) 20.2 g Zn; 93.7%
10) 6.34 tons $Al_2(SO_4)_3$
11) 0.404 g $Zn(OH)_2$
12) 0.793 g $BaCl_2$
13) 0.145 g Al in sample; 77.5% pure
14) $BaCl_2$ is limiting; 16.8 g $BaSO_4$
15) NaCl is limiting; 6.18 g AgCl
16) $ZnCl_2$ is limiting; 3.36 g Zn
17) 2.47 g $Al_2(SO_4)_3$
18) 0.3885 g Ag_2SO_4 in sample; 73.68% pure
19) 6.28 g $AlCl_3$
20) 3.49 g $BaSO_4$