Chemistry 1314 – Lecture Outline and Notes
Text: Chemistry – The Central Science, 10th edition, Brown, LeMay and Bursten

<u>Chapter 3. Stoichiometry: Calculations with Chemical Formulas and Equations</u>

Chemical Equations:

$2H_2 + O_2 \rightarrow 2H_2O$

This is a chemical equation

H_2 and O_2 are reactants

H_2O is the product

<u>Remember</u> – atoms are neither created nor destroyed. So, we must make sure the same number of atoms exists on both sides of the equation.

4 hydrogen on left and 4 hydrogen on right

2 oxygen on left and 2 oxygen on right

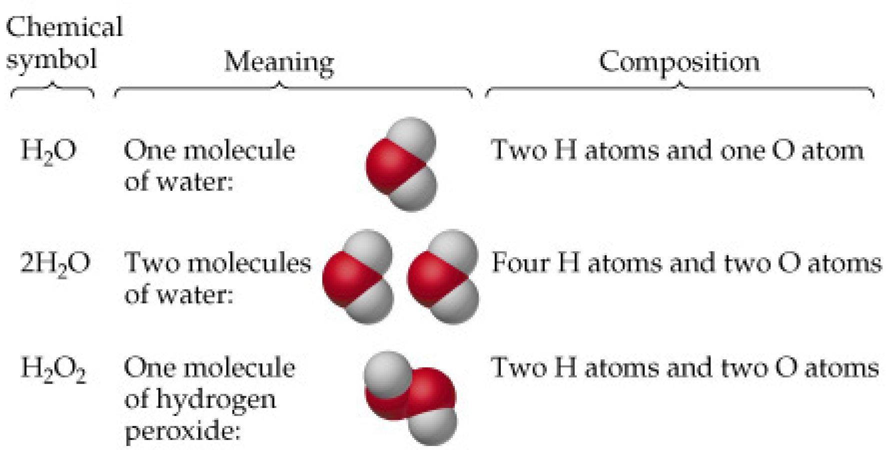
We say the equation is balanced!

So – let's take a closer look

$H_2 + O_2 \rightarrow H_2O$

This just shows the reactants and products, but it is not balanced.

We cannot alter the subscripts to balance because that changes the character of the components
Example $H_2 + O_2 \rightarrow H_2O_2$
H_2O_2 is a very different molecule than H_2O



In order to balance, we must add more components

$H_2 \quad + \quad O_2 \quad \rightarrow \quad H_2O$

First, let us look at Hydrogen – 2 on left and 2 on right. This is balanced.
BUT – if we look at oxygen – 2 on left and one on right

To balance, we double the amount of H_2O

$H_2 \quad + \quad O_2 \quad \rightarrow \quad \underline{2}H_2O$

The oxygens are balanced, but now the hydrogens are not: 2 on left and 4 on right, so we double the amount of hydgrogen

$\underline{2}H_2 + O_2 \rightarrow 2H_2O$

It is balanced!

$CH_4 + O_2 \rightarrow CO_2 + H_2O$

We usually start by balancing the elements in the fewest components. In this case we could start with either carbon or hydrogen.

Let's look at carbon – 1 on left and 1 on right – it is balanced.

Now for hydrogen – 4 on left and 2 on right

$CH_4 + O_2 \rightarrow CO_2 + \underline{2}H_2O$ (still unbalanced)

Now, check the oxygen – 2 on left and 4 on right

$CH_4 + \underline{2}O_2 \rightarrow CO_2 + \underline{2}H_2O$

This is now balanced!

We can also include more information, such as the states of the components.

$CH_4\ \underline{(g)} + 2O_2\ \underline{(g)} \rightarrow CO_2\ \underline{(g)} + 2H_2O\ \underline{(g)}$

Another example:

$CH_3OH + O_2 \rightarrow CO_2 + H_2O$

This equation is an example of combustion in air – the methanol will burn in oxygen to produce carbon dioxide and water. Therefore, it is a reaction with <u>oxygen</u> that produces a flame.

If a flame is produced, it is combustion.

We burn a hydrocarbon (a compound made from carbon and oxygen) to get CO_2 and H_2O.

Some simple patterns of reactions:

- Combination reactions:
  - $A + B \rightarrow C$
  - $C\ (s) + O_2\ (g) \rightarrow CO_2\ (g)$
- Decomposition reactions:
  - $C \rightarrow A + B$
  - $2KClO_3\ (s) \rightarrow 2KCl\ (s) + 3O_2\ (g)$

Formula & Molecular weights

Formula weight is the sum of the atomic weights of each atom in the chemical formula

FW of H_2SO_4 = 2(AW of H) + (AW of S) + 4(AW of O)
= 2(1.0 amu) + 32.1 amu + 4(16.0 amu)
= 98.1 amu

If the chemical formula represents a molecule, then the formula weight is also called the molecular weight.

MW of $C_6H_{12}O_6$ (glucose) =

Percentage composition from formulas

This is simply how much in percent does an element contribute to the compound

$$\%element = \frac{(number\_of\_atoms\_of\_element)(AW\_of\_element)}{FW\_of\_compound} \text{ x } 100\%$$

The percent carbon in glucose

% element =

For hydrogen:

% element =

And for oxygen

% element =

Now if we add the percent compositions of each element

The Mole

Not the blind fuzzy mammal!

A mole is a quantity – like a dozen (12) or a gross (144)

A mole is defined as the number of atoms in exactly 12 g of isotopically pure ^{12}C.

This is a very large number: 6.0221421×10^{23}

We call this number Avogadro's number

Therefore:

1 mol of ^{12}C atoms = 6.022×10^{23} ^{12}C atoms
1 mol of H_2O molecules = 6.022×10^{23} H_2O molecules
1 mol of NO_3^- ions = 6.022×10^{23} NO_3^- ions

Arrange the following in increasing number of O atoms:

1 mol H_2O; 1 mol CO_2; 3×10^{23} molecules of O_3
ANS:

This tells us that 1 mol of H_2O has 6.02 x 10^{23} molecules of H_2O, but how many atoms of H and O are in 1 mole of H_2O? H_2O is composed of 2 H atoms and 1 O atoms, therefore, 1 mole of H_2O would have 2(6.022 x 10^{23}) = 1.204 x 10^{24} atoms of H, but only 6.022 x 10^{23} atoms of O.

Another example:
How many oxygen atoms are in (a) 0.25 mol $Ca(NO_3)_2$ and (b) 1.50 mol of sodium carbonate.
a)

b)

Molar Mass
A mole is always the same number (6.022 x 10^{23}), but a mole of different things will clearly have a different mass. Example, ^{12}C has a mass of 12 amu, but ^{24}Mg has a mass of 24 amu, so a mole of ^{24}Mg would have twice the mass of ^{12}C.

1 mol of ^{12}C has a mass of 12g – by definition. We can extend this concept and see that
1 mol of ^{24}Mg has a mass of 24 g!

Therefore: The mass of one atom of an element (in amu) is numerically equivalent to the mass (in grams) of one mol of that element.
SO: 1 atom of ^{12}C has a mass of 12 amu ---- 1 mol ^{12}C has a mass of 12 g
1 atom of Cl has an average mass of 35.5 amu --- 1 mol Cl has a mass of 35.5 g

We can extend this to compounds.
1 H_2O molecule has a mass of 18.0 amu --- 1 mol H_2O has a mass of 18.0 g
1 NO_3^- ion has a mass of 62.0 amu --- 1 mol NO_3^- has a mass of 62.0 g

We call the mass in grams of 1 mol of substance (or g/mol) as the **molar mass** of the substance. The molar mass of any substance is always numerically equivalent to its formula weight in amu.

What is the formula weight of glucose, $C_6H_{12}O_6$?

So, what would its molar mass be =

Interconverting masses, moles, and number of particles.
Example: How many moles of sodium bicarbonate ($NaHCO_3$ – or sodium hydrogen carbonate) are there in 508 g of $NaHCO_3$?

Calculate the mass of 0.655 mol of $NaHCO_3$?

How many oxygen atoms are in 55.0 g of $NaHCO_3$?

Empirical Formulas from Analysis

The empirical formula tells the relative number of atoms each element contains.

Thus H_2O contains 2 H atoms to 1 O atom.

This applies to the molar level, thus 1 mol of H_2O contains 2 mol of H atoms and 1 mol of O atoms.

The ratio gives the subscripts of the compounds empirical formula. We can use the mole concept to determine the empirical formulas of chemical substances.

Mercury and chlorine form a compound with 73.9% Hg and 26.1% Cl, by mass. If we had a 100.0 g sample, it would contain 73.9 g of Hg and 26.1 g of Cl. We then use the molar masses to determine the number of moles of each element in our mercury and chlorine sample.

Molecular formula from empirical formula

The formula from percentage compositions is always the empirical formula. We can obtain the molecular formula if we know its molecular weight. NOTE: the subscripts in the molecular formula are always whole number multiples of the subscripts in the empirical formula. This multiple is found by comparing the ratio of the mass from the empirical formula with that of the mass from the molecular formula.

Example:

Ascorbic acid (vitamin C) contains 40.92% C, 4.58% H, and 54.50% O by mass. a) What is the empirical formula of ascorbic acid? b) It was experimentally determined that the molecular weight of ascorbic acid is 176 amu, what is its molecular formula?

Answer:

a)

b)

Combustion Analysis
Combustion analysis is a means of determining the amount of H_2O and CO_2 produced from the complete combustion of a hydrocarbon.
Example:
Isopropyl alcohol is composed of C, H, and O. Combustion of 0.255 g of isopropyl alcohol produces 0.561 g CO_2 and 0.306 g H_2O. What is the empirical formula of isopropyl alcohol?
Answer:

Quantitative Information from Balanced Equations:
Take the balanced equation:

$$2H_2\ (g) + O_2\ (g) \rightarrow 2H_2O\ (g)$$

This not only tells us that 2 molecules of hydrogen reacts with one molecule of oxygen to form 2 molecules of water, but it also says that 2 mol H_2 reacts with 1 mol O_2 to form 2 mol H_2O.

$$2\ \text{mol}\ H_2 \simeq 1\ \text{mol}\ O_2 \simeq 2\ \text{mol}\ H_2O$$

The symbol means "stoichiometrically equivalent"
We can use this stoichiometric information to determine information such as how many moles of H_2O can be formed from 1.57 mol O_2.

Limiting Reactions
A limiting reaction is when one reactant is used up before the other and, therefore, the limiting reactant limits the amount of product obtained.
For example, suppose we have 10 mol H_2 and 7 mol O_2. The reaction:

$$2H_2\ (g) + O_2\ (g) \rightarrow 2H_2O\ (g)$$

would suggest that we would need

moles of O = 10 mol H_2(1 mol O_2 /2 mol H_2) = 5 mol O_2.

Therefore, we will have 2 mol O_2 remaining after the reaction.
H_2 is the limiting reactant or limiting reagent.
O_2 is the excess reactant or excess reagent.

The quantity of product that is calculated to form when all the limiting reactant reacts is called the **theoretical yield**. The **percentage yield** relates the actual yield to the theoretical yield.

Percent yield = (actual yield / theoretical yield) x 100%