Chemical Calculations

Molar mass

The molar mass of a substance can be calculated from its formula and the atomic masses (from the periodic table) of the atoms contained in each *formula unit* of the substance (a formula unit of water for example is one molecule whereas one formula unit of sodium chloride would be one sodium ion and one chloride ion).

A *mole* is an amount of substance, where one mole (1 mol) of a substance will have its molar mass in grams, for example:

Molar mass of $Fe_2(CO_3)_3$:
2 Fe = 2x55.85 =111.7
3 C = 3x12.01 = 36.03
9 O = 9x16 = 144
= <u>291.73</u>
The 'molar mass' is the mass per mole, so the molar mass of iron carbonate is 291.7 g mol^{-1}
So 1 mol of iron carbonate has a mass of 291.7g

One mole of any substance has 6.02×10^{23} molecules (or formula units) of that substance. This number is called "Avagadro's number".

So there are 12.04×10^{23} Fe ions and 18.06×10^{23} carbonate ions in 291.7g of iron carbonate.

Mole calculations

To calculate the number of moles in some mass of substance or the mass of some amount of moles, we use this equation:

$$n = \frac{m}{M}$$

mass in grams (g)

molar mass in grams per mole (g mol^{-1})
[from the periodic table]

number of moles (mol)

This can be rearranged to $m = n \times M$

Another way of thinking about this relationship is:

$$\text{grams} \underset{\times M}{\overset{\div M}{\rightleftarrows}} \text{moles}$$

Mole ratio
A mole ratio is a fraction made from the coefficients (the number before each species in the balanced chemical equation) that represents the moles of each species required to exactly react, or the moles that will be produced.

Example: $2A + B \rightarrow A_2B$

Some of the mole ratios here are:

$$\frac{n_B}{n_A} = \frac{1}{2}$$

$$\frac{n_{A_2B}}{n_B} = \frac{1}{1}$$

Note: The mole ratio is the **only** time in chemical calculations that the coefficients are used.

Excess and limiting reactants
When a reaction occurs there is often not exactly the right amount of each reactant present. One reactant will be completely used up (this is called the **limiting** reactant) and the other reactant will have some left over (in **excess**).

To determine which reactant is limiting and which is excess:

1. Calculate moles **present** of each reactant (if this is already given, skip this step)
2. Calculate moles of one **required** to exactly react with the moles present of the other
   Do this by writing the mole ratio and rearranging to find the unknown.
3. **Compare** moles present with moles required.

Example: Given 1.0 g of H_2 and 10.0 g of O_2, determine which is excess and limiting for this reaction: $2H_2 + O_2 \rightarrow 2H_2O$

Moles **present**:

$$n_{H_2} = \frac{m_{H_2}}{M_{H_2}} = \frac{1.0}{2.016} = 0.50 \text{ mol} \qquad n_{O_2} = \frac{m_{O_2}}{M_{O_2}} = \frac{10.0}{32.00} = 0.31 \text{ mol}$$

Moles of O_2 **required** to react with the H_2 present:

$$\frac{n_{O_2}}{n_{H_2}} = \frac{1}{2}$$

$$\begin{aligned} \therefore n_{O_2} &= \frac{1}{2} \times n_{H_2} \\ &= \frac{1}{2} \times 0.50 \\ &= 0.25 \text{ mol} \end{aligned}$$

Compare with moles present of O_2:
There are 0.25 mol O_2 required and 0.31 mol O_2 present.
More moles are present than required, so <u>O_2 is excess</u>. This means <u>H_2 is limiting</u>.