• YIELD CALCULATIONS

The efficiency of a chemical transformation is usually expressed in terms of the **yield** of the reaction. Note that while reactions are rarely 100% efficient due to losses from side reactions or equilibration *etc*., students often get yields in excess of 100% indicating that the products are impure. For crystalline samples this is often because the crystals are "wet" i.e. they also contain the recrystallisation solvent, and the crystals just need to be left to dry further and then reweighed.

The **actual yield** is simply the mass of product obtained (usually expressed in grams). The **theoretical yield** is the maximum amount of product that could have been obtained if the reaction had been 100% efficient.

In order to determine the theoretical yield, one first needs to consider the stoichiometry of the balanced equation for the reaction and the number of moles of each reagent being used. From this, the reagent which is present in the lesser amount (in moles) when the stoichiometry is considered controls the amount of product that can be obtained. This reagent is called the **limiting reagent** as it dictates the *maximum* number of moles of product that can be obtained.

The **percentage yield** can be calculated using grams or moles (they are mathematically equivalent). It is simply the ratio of the amount of product actually obtained to the maximum amount of product possible:

% yield = 100 x (actual yield of product in g / theoretical yield of product in g)

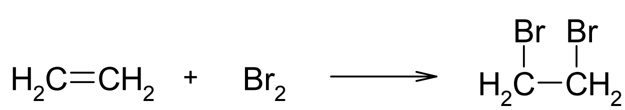
or

% yield = 100 x (moles of product obtained / maximum number of moles of product possible)

Note that if a synthesis is a linear multistep process, then the overall yield is the product of the yields of each step. So for example, if a synthesis has two steps, each of yield 50% then the overall yield is 50% x 50% = 25%.

Examples:
Here are two examples that illustrate the key issues. They are described in moles to make the contrast as obvious as possible:

(1) Ethene (0.05 moles) was reacted with bromine (0.06 moles) to give 1,2-dibromoethane (0.04 moles)



This equation is balanced, one molecule of alkene reacts with one molecule of bromine to give one molecule of product. Therefore, the alkene is the limiting reagent and the maximum number of moles of product that can be obtained is 0.05 moles. Hence the yield is 0.04 / 0.05 = 80%.

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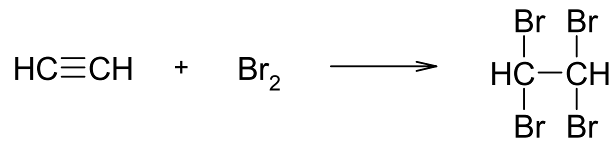
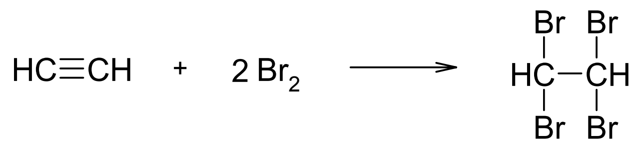
(2) Ethyne (0.05 moles) was reacted with bromine (0.06 moles) to give 1,1,2,2-dibromoethane (0.03 moles)



This equation is *not yet balanced* since *one* molecule of alkyne reacts with *two* molecule of bromine to give one molecule of product, so the balanced equation is:



Therefore, the bromine is the limiting reagent because there are only 0.06 / 2 = 0.03 moles of bromine to react with 0.05 moles of the alkene. This means that the maximum number of moles of product that can be obtained is 0.03 moles. Hence the yield is 0.03 / 0.03 = 100%.

Notice that the yield of the second reaction is higher than the yield of the first reaction despite the fact that the same amount of starting materials were used and less product was obtained!