Stoichiometric calculations

The limiting reagent

When two or more substances combine in a chemical reaction, the initial amount of one of those substances, the limiting reagent, determines the maximum amount of product that can form. Starting materials other than the limiting reagent are said to be present in excess.

There are two ways to determine which reagent is limiting and which reagents are present in excess: both methods require knowing the balanced reaction and the amounts of all starting materials in moles or grams present at the start of the reaction.

Method 1: Example

In this method the limiting reagent is the substance that can be totally used up in the course of the reaction. Consider the balanced equation

$$3\ LiAlH_4 + 4\ BF_3 \rightarrow 3\ LiF + 3\ AlF_3 + 2\ B_2H_6$$

and suppose that 50.00 g of $LiAlH_4$ ($\mathcal{M}$ = 37.95 g/mol) is brought into contact with 100.00 g of BF_3 ($\mathcal{M}$ = 67.81 g/mol).

Let's calculate how much $LiAlH_4$ is needed for all 100.00 g of BF_3 to react:

$$\left(\frac{100.00\text{ g }BF_3}{}\right)\left(\frac{\text{mol }BF_3}{67.81\text{ g }BF_3}\right)\left(\frac{3\text{ mol }LiAlH_4}{4\text{ mol }BF_3}\right)\left(\frac{37.95\text{ g }LiAlH_4}{\text{mol }LiAlH_4}\right)=41.97\text{ g }LiAlH_4$$

The 50.00-g supply of $LiAlH_4$ on hand is more than enough to react with all the BF_3. Thus, $LiAlH_4$ is present in excess and BF_3 is the limiting reagent.

Now let's calculate how much BF_3 is required for all 50.00 g of $LiAlH_4$ to react:

$$\left(\frac{50.00\text{ g }LiAlH_4}{}\right)\left(\frac{\text{mol }LiAlH_4}{37.95\text{ g }LiAlH_4}\right)\left(\frac{4\text{ mol }BF_3}{3\text{ mol }LiAlH_4}\right)\left(\frac{67.81\text{ g }BF_3}{\text{mol }BF_3}\right)=119.1\text{ g }BF_3$$

The 100.00-g supply of BF_3 is not sufficient for all the $LiAlH_4$ to react: some $LiAlH_4$ will be left over at the end of the reaction, once again demonstrating that $LiAlH_4$ is present in excess and that BF_3 is the limiting reagent.

Method 2: Example

In this method the limiting reagent is that substance that produces the least amount (in grams or moles) of product. Let's return to the balanced equation

$$3\ LiAlH_4 + 4\ BF_3 \rightarrow 3\ LiF + 3\ AlF_3 + 2\ B_2H_6$$

and again suppose that 50.00 g of $LiAlH_4$ is mixed with 100.00 g of BF_3. We now, of the three reaction products, arbitrarily choose LiF ($\mathcal{M}$ = 25.94 g/mol) and calculate the amount of this product that can form. We could equally well have chosen to calculate how much AlF_3 or B_2H_6 can form.

The amount of BF_3 initially present can produce

$$\left(\frac{100.00\text{ g }BF_3}{}\right)\left(\frac{\text{mol }BF_3}{67.81\text{ g }BF_3}\right)\left(\frac{3\text{ mol LiF}}{4\text{ mol }BF_3}\right)\left(\frac{25.94\text{ g LiF}}{\text{mol LiF}}\right)=28.69\text{ g LiF}$$

whereas the initial amount of $LiAlH_4$ can produce

$$\left(\frac{50.00\text{ g }LiAlH_4}{}\right)\left(\frac{\text{mol }LiAlH_4}{37.95\text{ g }LiAlH_4}\right)\left(\frac{3\text{ mol LiF}}{3\text{ mol }LiAlH_4}\right)\left(\frac{25.94\text{ g LiF}}{\text{mol LiF}}\right)=34.18\text{ g LiF}$$

We again conclude that BF_3 is the limiting reagent: the amount of BF_3 initially present produces less product than the amount of $LiAlH_4$ initially present produces.

Yields of chemical reactions

The theoretical yield of a reaction is the amount of product in grams or moles that forms if all of the limiting reagent is consumed. In many cases, however, all of the limiting reagent is not consumed for a variety of reasons: the reactants may not have come into contact with each other for a sufficient period of time, the temperature may have been too high or too low, etc. The percent yield relates the actual amount of product obtained to the theoretical yield:

$$\%\ \text{yield} = \frac{\text{actual yield (in grams or moles)}}{\text{theoretical yield (in grams or moles)}} \times 100\%$$

Example

Let's return to the balanced equation

$$3\ LiAlH_4 + 4\ BF_3 \rightarrow 3\ LiF + 3\ AlF_3 + 2\ B_2H_6$$

and again suppose that 50.00 g of $LiAlH_4$ is mixed with 100.00 g of BF_3. We established previously that (1) BF_3 is the limiting reagent; (2) 28.69 g of LiF forms when all of the limiting reagent reacts. The theoretical yield of LiF is thus 28.69 g. Suppose, however, that only 8.44 g of LiF is actually obtained. The percent yield is thus

$$\%\ \text{yield} = \frac{8.44\ \text{g LiF}}{28.69\ \text{g LiF}} \times 100\% = 29.4\%$$