

Stoichiometric calculations

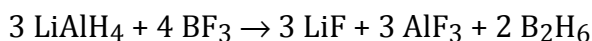
The limiting reagent

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



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

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

$$\left(\frac{100.00 \text{ g BF}_3}{67.81 \text{ g BF}_3}\right)\left(\frac{\text{mol BF}_3}{4 \text{ mol BF}_3}\right)\left(\frac{3 \text{ mol LiAlH}_4}{3 \text{ mol LiAlH}_4}\right)\left(\frac{37.95 \text{ g LiAlH}_4}{\text{mol LiAlH}_4}\right) = 41.97 \text{ g LiAlH}_4$$

The 50.00-g supply of LiAlH₄ on hand is more than enough to react with all the BF₃. Thus, LiAlH₄ is present in excess and BF₃ is the limiting reagent.

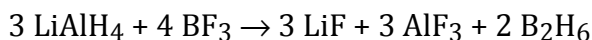
Now let's calculate how much BF₃ is required for all 50.00 g of LiAlH₄ to react:

$$\left(\frac{50.00 \text{ g LiAlH}_4}{37.95 \text{ g LiAlH}_4}\right)\left(\frac{\text{mol LiAlH}_4}{3 \text{ mol LiAlH}_4}\right)\left(\frac{4 \text{ mol BF}_3}{3 \text{ mol LiAlH}_4}\right)\left(\frac{67.81 \text{ g BF}_3}{\text{mol BF}_3}\right) = 119.1 \text{ g BF}_3$$

The 100.00-g supply of BF₃ is not sufficient for all the LiAlH₄ to react: some LiAlH₄ will be left over at the end of the reaction, once again demonstrating that LiAlH₄ is present in excess and that BF₃ 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



and again suppose that 50.00 g of LiAlH₄ is mixed with 100.00 g of BF₃. We now, of the three reaction products, arbitrarily choose LiF ($\mathcal{M} = 25.94 \text{ g/mol}$) and calculate the amount of this product that can form. We could equally well have chosen to calculate how much AlF₃ or B₂H₆ can form.

The amount of BF₃ initially present can produce

$$\left(\frac{100.00 \text{ g BF}_3}{67.81 \text{ g BF}_3}\right)\left(\frac{\text{mol BF}_3}{4 \text{ mol BF}_3}\right)\left(\frac{3 \text{ mol LiF}}{3 \text{ mol LiF}}\right)\left(\frac{25.94 \text{ g LiF}}{\text{mol LiF}}\right) = 28.69 \text{ g LiF}$$

whereas the initial amount of LiAlH₄ can produce

$$\left(\frac{50.00 \text{ g LiAlH}_4}{37.95 \text{ g LiAlH}_4}\right)\left(\frac{\text{mol LiAlH}_4}{3 \text{ mol LiAlH}_4}\right)\left(\frac{3 \text{ mol LiF}}{3 \text{ mol LiAlH}_4}\right)\left(\frac{25.94 \text{ g LiF}}{\text{mol LiF}}\right) = 34.18 \text{ g LiF}$$

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.

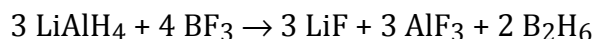
Yields of chemical reactions

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



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

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