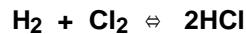


## Chemical Examples for Mass Action Law Applications

### Advanced

What can one do with the mass action law? A lot - but it is not always very obvious. Lets ask a few "dumb" questions and see how far we get.

First we look at a really simple reaction, e.g



To keep it easy, we start with equal amounts of  $\text{H}_2$  and  $\text{Cl}_2$ .

How much  $\text{HCl}$  do we get? Notice that we have [the same number of mols](#) on both sides of the reaction equation.

Well, in equilibrium (denoted by  $[\dots]$ ) we have

$$\frac{[\text{HCl}]^2}{[\text{H}_2] \cdot [\text{Cl}_2]} = K$$

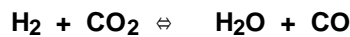
or, with  $[\text{H}_2] = [\text{Cl}_2] = [\text{equ}]$

$$[\text{HCl}] = [\text{equ}] \cdot K^{1/2}$$

One equation with two unknowns; not sufficient for calculating numbers.

But then we also have the condition that the number of the atoms involved stays constant, i.e.  $[\text{H}_2] + 2[\text{HCl}] = \text{constant} = \text{e.g. the number of } \text{H}_2 \text{ mols before the reaction.}$

Next, a little bit harder. Lets start with arbitrary concentrations of something and see what we can say about the *yield* of the reaction. For varieties sake lets look at



Again a simple reaction with the same number of mols on both sides, so we [do not have to worry](#) about the precise form of the mass action law.

We start with  $n^0_{\text{H}_2}$  and  $n^0_{\text{CO}_2}$  mols of the reacting gases and define as the *yield*  $y$  the number of mols of  $\text{H}_2\text{O}$  that the reaction will produce at equilibrium. This leaves us with

$$n_{\text{H}_2\text{O}} = y$$

$$n_{\text{CO}} = y$$

$$n_{\text{H}_2} = n^0_{\text{H}_2} - y = \text{equilibrium concentration of H}_2$$

$$n_{\text{CO}_2} = n^0_{\text{CO}_2} - y = \text{equilibrium concentration of CO}$$

$$\Sigma n = n^0 = n^0_{\text{H}_2} + n^0_{\text{CO}_2}$$

The last equation holds because the mol count never changes in this example.

The mass action law now gives

$$\frac{y^2}{(n_{\text{H}_2}^0 - y) \cdot (n_{\text{CO}_2}^0 - y)} = K$$

$$y = \left( \frac{1}{2} (1 - K) \right) \cdot \left( \left( -n^0 \cdot K \pm \left( (n^0 \cdot K)^2 + 4 \cdot (1 - K) \cdot n_{\text{H}_2}^0 \cdot (n^0 - n_{\text{H}_2}^0) \cdot K \right)^{1/2} \right) \right)$$

● The starting concentration of  $\text{CO}_2$ , i.e.  $n_{\text{CO}_2}$ , is expressed as  $n_{\text{CO}_2} = n^0 - n_{\text{H}_2}$ .

▸ Looks extremely messy, but this is just the standard solution for a second order equation. Whatever this solution means in detail, it tells us that the yield is a function of the starting concentrations of the ingredients.

● What kind of starting concentrations will give us *maximum* yield? To find out, we have to form  $dy/dn_{\text{H}_2}^0 = 0$ .

● Well, go through the math yourself; this is elementary stuff. The solution is

$$n_{\text{H}_2}^0 = \frac{n^0}{2}$$

$$n_{\text{CO}_2}^0 = \frac{n^0}{2} = n_{\text{H}_2}^0$$

▸ In other words: maximum yield is achieved if you mix just the right amounts of the starting stuff. This result is always true, even for more complicated reactions.

● At this point we stop, again because otherwise we might turn irreversibly into chemists.