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

$$H_2 + Cl_2 \Leftrightarrow 2HCl$$

- To keep it easy, we start with equal amounts of H_2 and Cl_2 .
- How much **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 **[..]**) we have

$$\frac{[HCl]^2}{[H_2] \cdot [Cl_2]} = K$$

- or, with $[H_2] = [Cl_2] = [equ]$

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

- 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. $[H_2] + 2[HCl] =$ constant = e.g. the number of H_2 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

$$H_2 + CO_2 \Leftrightarrow H_2O + CO$$

- 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_{H2} and n^0_{CO2} mols of the reacting gases and define as the *yield* y the number of mols of H_2O that the reaction will produce at equilibrium. This leaves us with

$$n_{H2O} = y$$

$$n_{CO} = y$$

$$n_{H2} = n^0_{H2} - y = \text{equilibrium concentration of } H_2$$

$$n_{CO2} = n^0_{CO2} - y = \text{equilibrium concentration of CO}$$

$$\Sigma n = n^0 = n^0_{H2} + n^0_{CO2}$$

- The last equation holds because the mol count never changes in this example.
- The mass action law now gives

$$\frac{y^2}{(n^0_{H2} - y)\cdot(n^0_{CO2} - y)} = K$$

$$y = \left(\frac{1}{2}\left(1 - K\right)\right)\cdot\left(\left(-n^0\cdot K \pm \left((n^0\cdot K)^2 + 4\cdot(1-K)\cdot n^0_{H2}\cdot(n^0 - n^0_{H2})\cdot K\right)^{1/2}\right)\right)$$

- The starting concentration of $\mathbf{CO_2}$, i.e n_{CO2}, is expressed as $n_{CO2} = n^0 - n^0_{H2}$.

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 $dy/dn^0_{H2} = 0$.
- Well, go through the math yourself; this is elementary stuff. The solution is

$$n^0_{H2} = \frac{n^0}{2}$$

$$n^0_{CO2} = \frac{n^0}{2} = n^0_{H2}$$

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.