18.1 – Calculations Involving Acids and Bases

18.1.1 - State the expression for the ionic product constant of water

The ionisation of water happens according to the equation:

$$H_2O_{(l)} \leftrightarrow H^+{}_{(aq)} + OH^-{}_{(aq)} \qquad \Delta H^\theta = +57.3 \; kJ \; mol^{-1}$$

Using this, we can find the expression of the equilibrium constant:

$$K_c = \frac{\left[H^+{}_{(aq)}\right] \times \left[OH^-{}_{(aq)}\right]}{\left[H_2O_{(l)}\right]}$$

However, the concentration of water is relatively constant, so it can be removed from the equation. This is because the equilibrium lies so far to the left that the change in concentration does not have a significant effect on the value of K_c. Therefore, it can be written as:

$$K_W = [H_3O^+][OH^-] = 1.00 \times 10^{-14} \; mol^2 \; dm^{-6} \; at \; 25°C$$

The dissociation of water is an endothermic reaction. As a result, the K_w value increases as the temperature increases.
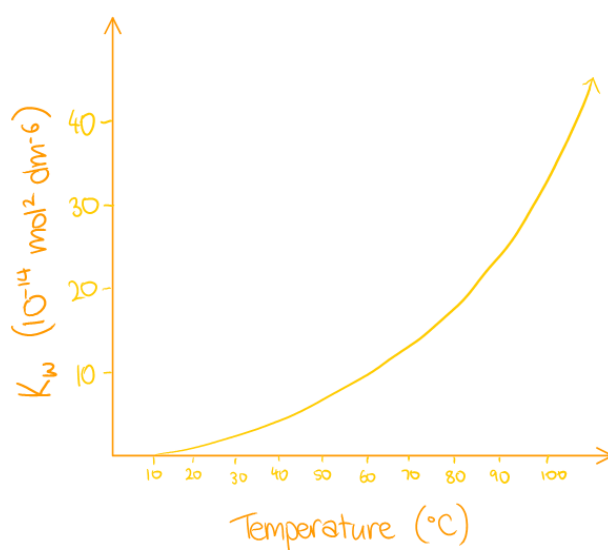
18.1.2 - Deduce [H⁺(aq)] and [OH⁻(aq)] for water at different temperatures given K_w values

Given a temperature and the value of K_w, we can calculate the value of [H⁺], using the equation:

$$K_w = [H^+][OH^-]$$

Since OH- and H+ are in equal ratios of 1:1, in pure water, [H⁺] = [OH⁻], so:

$$K_w = [H^+]^2$$
$$\sqrt{K_w} = [H^+]$$

[OH⁻] will be equal to [H⁺].

18.1.3 - Solve problems involving [H+(aq)], [OH-(aq)], pH and pOH

If the pH of a solution is <7, it is acidic. If the pH is >7, then it is alkaline. The pH of a solution is found according to the equation:

$$pH = -\log_{10}[H^+{}_{(aq)}]$$

Therefore, given the pH, the [H⁺] can be found using:

$$[H^+] = 10^{-pH}$$

Likewise, the pOH is found according to the equation:

$$pOH = -\log_{10}[OH^-{}_{(aq)}]$$

Given the pOH, the [OH⁻] can be determined:

$$[OH^-] = 10^{-pOH}$$

If you are given the concentration of a basic solution and need to find the pH, this can be done by rearranging the equation for K_w:

$$[H^+] = \frac{K_w}{[OH^-]}$$

The [H⁺] can then be used to find the pH.

Alternatively, if you are given the [OH⁻] and calculate the pOH, then pH can be found by:

$$pH = 14 - pOH$$

When you are given the equation for the reaction of a strong acid or base with water and the initial concentration of acid or base, then you can **assume complete dissociation**. This means that the $[H^+]$ or $[OH^-]$ will be equal to the initial concentration of acid or base. However, it is essential to check the stoichiometric ratio of acid-H^+ or base-OH^-, as this will need to be taken into account. For example, looking at a diprotic acid:

$$H_2SO_{4\,(aq)} + 2H_2O_{(l)} \rightarrow 2H_3O^+_{\,(aq)} + SO_4^{\,2-}_{\,(aq)}$$

The concentration of $[H^+]$ (or $[H_3O^+]$) will be double the initial concentration of H_2SO_4.

Also, the pK_w can be calculated, given the K_w:

$$pK_w = -\log_{10} K_w$$

18.1.4 - State the equation for the reaction of any weak acid or weak base with water, and hence deduce the expressions for K_a and K_b

When a weak acid reacts with water, the reaction will favour the left-hand side of the equation and it will have a small equilibrium constant.

$$HA_{(aq)} + H_2O_{(l)} \leftrightarrow A^-_{\,(aq)} + H_3O^+_{\,(aq)}$$

The K_a is simply the K_c for the reaction multiplied by $[H_2O]$, so that it given the expression:

$$K_a = \frac{[A^-][H_3O^+]}{[HA]}$$

Likewise, if we are given a reaction for a weak base with water:

$$B_{(aq)} + H_2O_{(l)} \leftrightarrow HB^+_{\,(aq)} + OH^-_{\,(aq)}$$

The K_b is found the same way, giving the expression:

$$K_b = \frac{[HB^+][OH^-]}{[B]}$$

You will only ever be asked about reactions involving the transfer of one proton

18.1.5 - Solve problems involving solutions of weak acids and bases using the expressions:

In reactions of weak acids and bases, we cannot make the same assumptions as for the dissociation of strong acids and bases. Instead, we must use the relationships below.

For a weak acid and its conjugate base, the equation below can be used:

$$K_w = K_a \times K_b$$

By finding the $-\log_{10}$ of these, this means that:

$$pK_w = pK_a + pK_b$$

We can assume in these reactions that **[acid]$_{initial}$ ≈ [acid]$_{equilibrium}$** since there is so little dissociation of the acid. Also, given that the acid is monoprotic, then **[A$^-$] = [H$_3$O$^+$]**. Using these relationships, we can say that:

$$K_a = \frac{[H_3O^+]^2}{[HA]}$$

Therefore: $[H_3O^+] = \sqrt{K_a \times [HA]}$, which can then be used to calculate pH.

Remember to state the assumptions:

- [acid]$_{initial}$ ≈ [acid]$_{equilibrium}$
- [A$^-$] = [H$_3$O$^+$]
- There is negligible self-ionisation of the water so the [H$_3$O$^+$] is not affected
- The temperature is 25°C

Another relationship that can be used is:

$$pK_w = pH + pOH$$

Remember the IB will not ask you to use quadratic equations.

18.1.6 - Identify the relative strengths of acids and bases using values of K_a, K_b, pK_a and pK_b

The pK_a or pK_b is found using the equations:

$$pK_a = -\log_{10} K_a$$

$$pK_b = -\log_{10} K_b$$

Since they have a logarithmic relationship, a weaker acid will have a small K_a value but a larger pK_a value. Likewise, a weak base will have a small K_b but a large pK_b.

You will often be asked to compare between a number of acids or base to determine which is strongest or weakest.