Cambridge (CIE) A Level Chemistry

Your notes

Partition Coefficients

Contents

* Partition Coefficients

Your notes

The Partition Coefficient

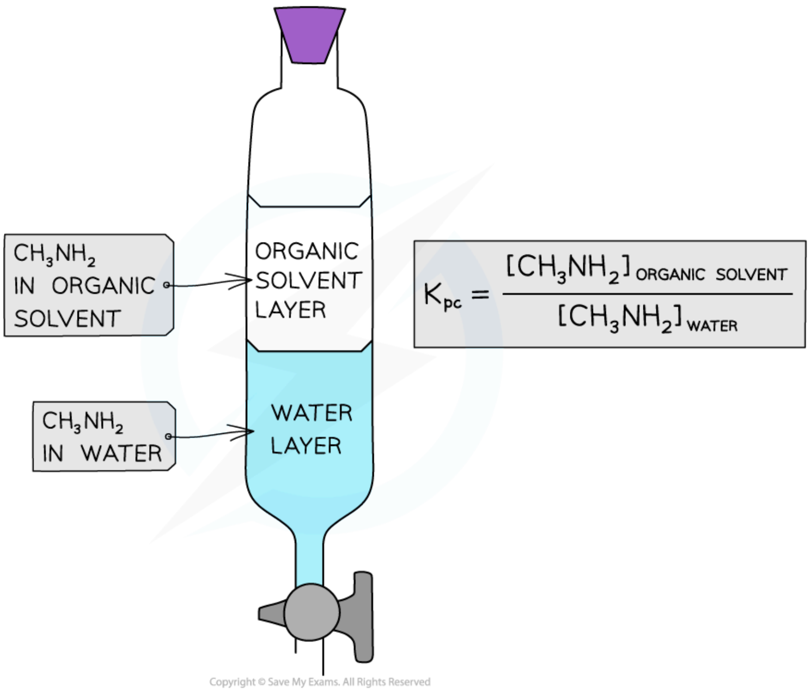
- The **partition coefficient (K_{pc})** is the ratio of the concentrations of a **solute** in two different immiscible solvents in contact with each other when equilibrium has been established (at a particular temperature)
- For example, **methylamine (CH_3NH_2)** is dissolved in two immiscible solvents:
  - Water
  - An organic solvent
- A **separating funnel** is shaken with the organic solvent and aqueous methylamine
- The methylamine is **soluble** in both solvents, so when the mixture is left to settle an **equilibrium** is established
  - The **rate** of methylamine molecules moving from the organic layer into the aqueous layer is **equal** to the rate of molecules moving from the aqueous layer to the organic layer

$$CH_3NH_2\,(aq) \rightleftharpoons CH_3NH_2\,(organic\ solvent)$$

- The value of its **equilibrium constant** is also called the **partition coefficient**

$$K_{pc} = \frac{[CH_3NH_2\,(organic\ \ solvent)]}{[CH_3NH_2\,(aq)]}$$

Defining the partition coefficient



The partition coefficient is the ratio of methylamine molecules in the organic and aqueous layer once equilibrium has been established

Your notes

Partition Coefficient Calculations

- The **partition coefficient** (K_{pc}) for a system in which the solute is in the same physical state in the two solvents can be calculated using the equilibrium expression

Worked Example

Calculating the partition coefficient

100 cm^3 of a 0.150 mol dm^{-3} solution of aqueous methylamine (CH_3NH_2) was shaken with 75.0 cm^3 of an organic solvent at 25 °C and left in the separating funnel to allow an equilibrium to be established.

Only 50.0 cm^3 of the aqueous layer was run off and titrated against 0.225 mol dm^{-3} dilute hydrochloric acid (HCl) with an end-point of 14.1 cm^3 of HCl.

Calculate the partition coefficient of methylamine between the organic solvent and water.

Answer

- **Step 1:** Write down the equilibrium equation:

$$CH_3NH_2\,(aq) \rightleftharpoons CH_3NH_2\,(organic\ solvent)$$

- **Step 2:** Write down the equilibrium expression:

$$K_{pc} = \frac{[CH_3NH_2\,(organic\quad solvent)]}{[CH_3NH_2\,(aq)]}$$

- **Step 3:** Determine how many moles of CH_3NH_2 have reacted with HCl at the end-point:
  - At the **end-point,** all CH_3NH_2 (aq) has been neutralised by HCl (aq)

$$CH_3NH_2\,(aq) + HCl\,(aq) \rightarrow CH_3NH_3Cl\,(aq)$$

- CH_3NH_2 and HCl react in a ratio of 1:1

$$Mol\,(HCl) = mol\,(CH_3NH_2) = 0.225 \times 0.0141$$

$$Mol\,(CH_3NH_2) = 3.1725 \times 10^{-3}\ mol$$

- **Step 4:** Determine the number of moles of CH_3NH_2 present in the aqueous layer:
  - Only 50.0 cm^3 of the aqueous layer was used to titrate against HCl
  - Thus, 3.1725×10^{-3} mol of CH_3NH_2 was present in only 50.0 cm^3 of the aqueous layer
  - The number of moles of CH_3NH_2 in 100 cm^3 **aqueous layer** is, therefore:

$$Mol\,(CH_3NH_2\ aqueous\ layer) = 3.1725 \times 10^{-3} \times 2 = 6.345 \times 10^{-3}\ mol$$

- **Step 5:** Determine the number of moles of CH_3NH_2 in the organic layer:

Your notes

$$\text{Mol } CH_3NH_2 \text{ (organic layer)} = \text{mol } CH_3NH_2 \text{ (total)} - \text{mol } CH_3NH_2 \text{ (aqueous layer)}$$

$$\text{Mol } CH_3NH_2 \text{ (total)} = 0.100 \times 0.150 = 0.015 \text{ mol}$$

$$\text{Mol } CH_3NH_2 \text{ (organic layer)} = 0.015 - 6.345 \times 10^{-3}$$

$$\text{Mol } CH_3NH_2 \text{ (organic layer)} = 8.655 \times 10^{-3} \text{ mol}$$

- **Step 6:** Change the number of moles into **concentrations:**
  - Aqueous layer:

$$\text{Concentration } (CH_3NH_2 \text{ in aqueous layer}) = \frac{6.345 \times 10^{-3}}{0.100}$$

$$\text{Concentration } (CH_3NH_2 \text{ in aqueous layer}) = 0.06345 \text{ mol dm}^{-3}$$

- Organic layer:

$$\text{Concentration } (CH_3NH_2 \text{ in organic layer}) = \frac{8.655 \times 10^{-3}}{0.075}$$

$$\text{Concentration } (CH_3NH_2 \text{ in organic layer}) = 0.1154 \text{ mol dm}^{-3}$$

- **Step 7:** Substitute the values into the K_{pc} expression:

$$K_{pc} = \frac{0.1154}{0.06345}$$

$$K_{pc} = 1.82$$

- Since the value of K_{pc} is **larger than 1**, methylamine is more soluble in the organic solvent than in water

Factors Affecting the Partition Coefficient

- The partition coefficient (K_{pc}) depends on the **solubilities** of the **solute** in the two **solvents**
- The degree of solubility of a solute is determined by how strong the **intermolecular bonds** between **solute** and **solvent** are
- The strength of these intermolecular bonds, in turn, depends on the **polarity** of the **solute** and **solvent molecules**
- For example, ammonia is more soluble in water than in an organic solvent such as carbon tetrachloride (CCl_4)
  - Ammonia and water are both polar molecules that form **hydrogen bonds** with each other
  - Ammonia forms **permanent dipole-induced dipole** forces with the non-polar CCl_4 molecules
  - Since these forces are **much** weaker than hydrogen bonding, ammonia is **less soluble** in CCl_4

- When K_{pc} is < 1 the **solute** is more soluble in water than the organic solvent
- When K_{pc} is > 1 the **solute** is more soluble in the organic solvent than the water

Your notes