

Reactivity 2.3 HL

IB CHEMISTRY HL

<p>25 Mn Manganese 54.938045</p>	<p>16 S Sulfur 32.065</p>	<p>J</p>	<p>6 C Carbon 12.0107</p>	<p>2 He Helium 4.002602</p>	<p>25 Mn Manganese 54.938045</p>
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Reactivity 2.3.5

Understandings:

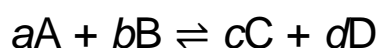
- The reaction quotient, Q , is calculated using the equilibrium expression with non-equilibrium concentrations of reactants and products.

Learning outcomes:

- Calculate the reaction quotient Q from the concentrations of reactants and products at a particular time, and determine the direction in which the reaction will proceed to reach equilibrium.

Reaction quotient Q

- The reaction quotient Q measures the relative amounts of reactants and products at a certain point in time.
- It is expressed with non-equilibrium concentrations of reactants and products.



$$Q = \frac{[C]^c [D]^d}{[A]^a [B]^b}$$

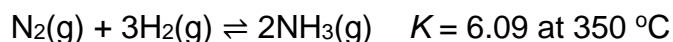
Exercise: Outline the difference between the reaction quotient Q and the equilibrium constant K .

The reaction quotient Q is calculated using non-equilibrium concentrations of reactants and products. The equilibrium constant K is calculated using equilibrium concentrations of reactants and products.

Q , K and direction of reaction

- When the value of Q is equal to the value of K ($Q = K$) the reaction is at equilibrium.
- If the value of Q is lower than the value of K ($Q < K$) the concentration of products is lower than at equilibrium.
- The reaction will proceed to the right to increase the concentration of products and the value of Q until equilibrium is reached.
- If the value of Q is higher than the value of K ($Q > K$) the concentration of products is higher than at equilibrium.
- The reaction will proceed to the left to decrease the concentration of the products and the value of Q until equilibrium is reached.

Example 1: Calculate the value of Q when $[\text{N}_2]$ is $0.814 \text{ mol dm}^{-3}$, $[\text{H}_2]$ is 0.422 and $[\text{NH}_3]$ is $0.372 \text{ mol dm}^{-3}$.

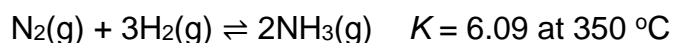


$$Q = \frac{[0.372]^2}{[0.814][0.422]^3} = 2.26$$

Based on your calculation, predict in which direction the reaction will proceed to reach equilibrium and explain your answer.

$Q < K_c$ so the reaction will proceed to the right to reach equilibrium.

Example 2: Calculate the value of Q when $[\text{N}_2]$ is $0.814 \text{ mol dm}^{-3}$, $[\text{H}_2]$ is 0.523 and $[\text{NH}_3]$ is 1.32 mol dm^{-3} .



$$Q = \frac{[1.32]^2}{[0.841][0.523]^3} = 14.5$$

Based on your calculation, predict in which direction the reaction will proceed to reach equilibrium and explain your answer.

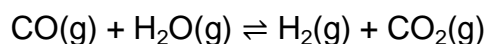
$Q > K_c$ – the reaction will proceed to the left to reach equilibrium.

Summary:

Q vs K	Direction of reaction
$Q > K$	Reaction proceeds to left (reactants side)
$Q < K$	Reaction proceeds to right (products side)
$Q = K$	No net change (reaction is at equilibrium)

Exercises:

- 1) The table below show non-equilibrium concentrations of reactions and products for the following reaction at 527 °C. The value of K for this reaction at 527 °C is 5.10.



Species	Concentration at time t (mol dm ⁻³)
CO(g)	0.15
H ₂ O(g)	0.25
H ₂ (g)	0.42
CO ₂ (g)	0.37

Calculate the reaction quotient Q and predict in which direction the reaction will proceed to reach equilibrium.

Write expression for Q :

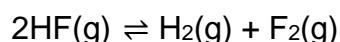
$$Q = \frac{[\text{H}_2][\text{CO}_2]}{[\text{H}_2\text{O}][\text{CO}]}$$

Input values into the expression (products in numerator, reactants in denominator)

$$Q = \frac{(0.42)(0.37)}{(0.25)(0.15)} = 4.1$$

The value of the reaction quotient Q is less than the value of K so the reaction will proceed to the right (products side), increasing the value of Q .

- 2) The table below shows non-equilibrium concentrations of reactions and products for the following reaction at 1000 °C. The value of K for this reaction at 1000 °C is 1.00×10^{-13} .



Species	Concentration at time t (mol dm ⁻³)
HF(g)	23.0
H ₂ (g)	0.540
F ₂ (g)	0.380

Calculate the reaction quotient Q and predict in which direction the reaction will proceed to reach equilibrium.

Write expression for Q :

$$Q = \frac{[\text{H}_2][\text{F}_2]}{[\text{HF}]^2}$$

Input values into the expression (products in numerator, reactants in denominator)

$$Q = \frac{(0.540)(0.380)}{(23.0)^2} = 3.88 \times 10^{-4}$$

The value of the reaction quotient Q is greater than the value of K so the reaction will proceed to the left (reactants side), decreasing the value of Q .

Reactivity 2.3.6

Understandings:

- The equilibrium law is the basis for quantifying the composition of an equilibrium mixture.

Learning outcomes:

- Solve problems involving values of K and initial and equilibrium concentrations of the components of an equilibrium mixture.

Additional notes:

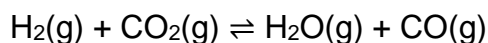
- When K is very small, the approximation $[\text{reactant}]_{\text{initial}} \approx [\text{reactant}]_{\text{eqm}}$ should be understood.
- The use of quadratic equations is not expected. Only homogeneous equilibria will be assessed.

Linking questions:

- Reactivity 3.1 How does the equilibrium law help us to determine the pH of a weak acid, weak base or a buffer solution?

Determining the value of K given the concentration of products and reactants at equilibrium

Example: Calculate the K for the reaction:



given the following equilibrium concentrations:

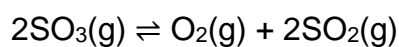
$$[\text{H}_2] = 0.61 \text{ mol dm}^{-3}, [\text{CO}_2] = 1.6 \text{ mol dm}^{-3}, [\text{H}_2\text{O}] = 1.1 \text{ mol dm}^{-3}, [\text{CO}] = 1.4 \text{ mol dm}^{-3}$$

Write the expression for the K and plug in the equilibrium concentrations;

$$K = (1.1 \times 1.4) \div (0.61 \times 1.6) = 1.6$$

Determining the value of K given the initial concentration of one species and the equilibrium concentration of another

Example: Before equilibrium is reached, a 1.00 dm³ flask contains 0.350 mol of SO₃(g) at 832° C. Determine the K for the reaction if 0.093 mol of oxygen is present at equilibrium.

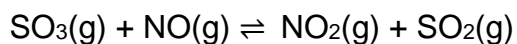


	2SO ₃ (g)	O ₂ (g)	2SO ₂ (g)
Initial (mol dm ⁻³)	0.350	0	0
Change (mol dm ⁻³)	-2 × 0.093	+0.093	+ 2 × 0.093
Equilibrium (mol dm ⁻³)	0.164	0.093	0.186

$$K = (0.093 \times 0.186^2) \div (0.164^2) = 0.12$$

Calculating the equilibrium concentrations given the K for the reaction and initial concentrations

The K for the following reaction is 6.78 at a certain temperature. The initial concentrations of NO and SO₃ are both 0.0300 mol dm⁻³. Calculate the equilibrium concentration of each reactant.



	SO ₃ (g)	NO(g)	NO ₂ (g)	SO ₂ (g)
Initial (mol dm ⁻³)	0.0300	0.0300	0	0
Change (mol dm ⁻³)	- x	- x	+ x	+ x
Equilibrium (mol dm ⁻³)	0.0300 - x	0.0300 - x	x	x

$$6.78 = (x^2) \div (0.0300 - x)^2$$

take the square root of both sides

$$2.60 = x \div (0.0300 - x)$$

Solve for x

$$x = 0.0217$$

$$[\text{SO}_3] = 0.0300 - 0.0217 = 0.00830 \text{ mol dm}^{-3}$$

$$[\text{NO}] = 0.0300 - 0.0217 = 0.00830 \text{ mol dm}^{-3}$$

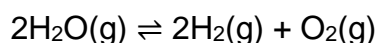
$$[\text{NO}_2] = 0.0217 \text{ mol dm}^{-3}$$

$$[\text{SO}_2] = 0.0217 \text{ mol dm}^{-3}$$

Calculating equilibrium concentrations when K_c is very small

- In some chemical reactions, K is a small value, less than 1×10^{-3} . In these reactions, the forward reaction barely proceeds, and the equilibrium mixture consists of mostly reactants.
- The change in the initial concentration of reactants is almost zero and the equilibrium concentrations of reactants are almost equal to their initial concentrations ($[\text{reactant}]_{\text{initial}} \approx [\text{reactant}]_{\text{eqm}}$).

Example: The thermal decomposition of water has a K value of 7.3×10^{-18} at 1000°C . If the initial concentration of H_2O is 0.10 mol dm^{-3} , calculate the concentration of O_2 at equilibrium.



	$2\text{H}_2\text{O}(\text{g})$	$2\text{H}_2(\text{g})$	$\text{O}_2(\text{g})$
Initial (mol dm^{-3})	0.10	0	0
Change (mol dm^{-3})	$-2x$	$+2x$	$+x$
Equilibrium (mol dm^{-3})	$0.10 - 2x$	$2x$	x

Because value of K is less than 1×10^{-3} , the equilibrium concentration of the H_2O is the same as the initial concentration ($[\text{reactant}]_{\text{initial}} \approx [\text{reactant}]_{\text{eqm}}$).

Solve for x

$$x = 2.6 \times 10^{-7}$$

Equilibrium concentration of $\text{H}_2 = 2x = 5.2 \times 10^{-7} \text{ mol dm}^{-3}$

The assumption made in this example is that subtracting x from the initial concentration will not make a difference within the precision used (to 2 significant figures). In general, if the value of K is less than 1×10^{-3} , this assumption is valid.

Reactivity 2.3.7

Understandings:

- The equilibrium constant and Gibbs energy change, ΔG , can both be used to measure the position of an equilibrium reaction.

Learning outcomes:

- Calculations using the equation $\Delta G^\ominus = -RT \ln K$.

Additional notes:

- The equation is given in the data booklet.

Linking questions:

- Reactivity 1.4 How can Gibbs energy be used to explain which of the forward or backward reaction is favoured before reaching equilibrium?

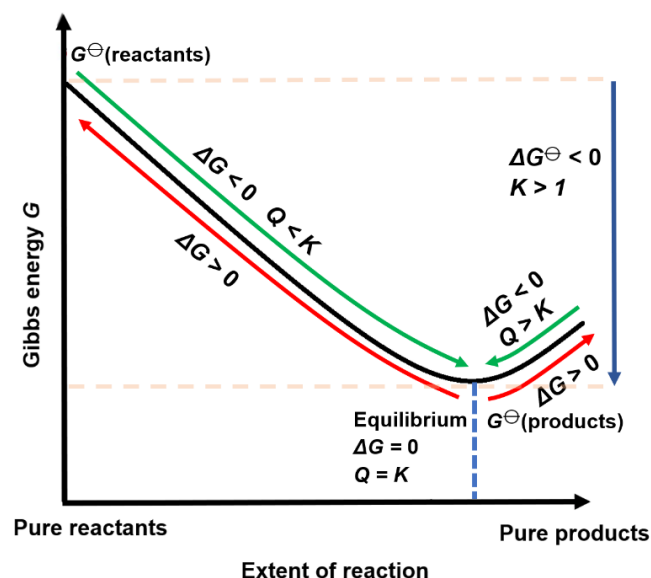
Gibbs free energy and equilibrium

- A system not at equilibrium (where $Q \neq K$) will proceed spontaneously in the direction necessary to reach equilibrium (where $Q = K$).
- As a reaction approaches equilibrium, the Gibbs free energy change, ΔG , becomes less negative and eventually reaches zero at equilibrium.
- The equilibrium position occurs where the free energy is at its minimum and entropy is at its maximum.

Plots of free energy against extent of reaction

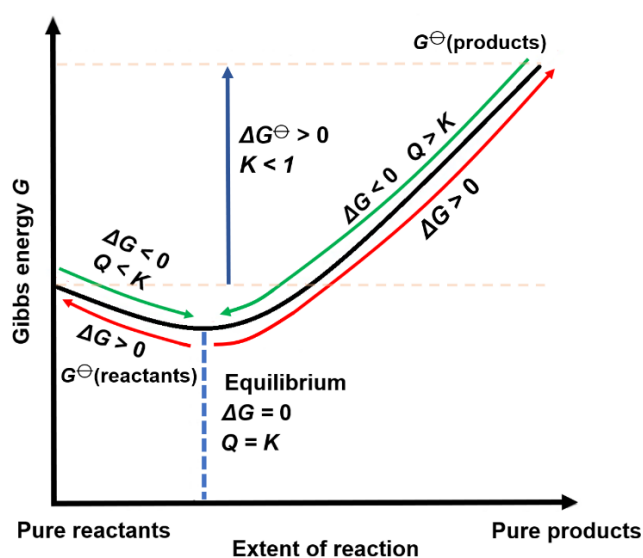
- The reaction proceeds spontaneously from either pure reactants or pure products to the equilibrium position where $\Delta G = 0$ and $Q = K$ (shown by the green arrows).
- The reaction away from the equilibrium position is non-spontaneous (shown by the red arrows).

Spontaneous reaction



For a spontaneous reaction, the equilibrium position lies further towards pure products meaning that at equilibrium $[\text{products}] > [\text{reactants}]$ and $K > 1$. $G^\ominus(\text{products}) < G^\ominus(\text{reactants})$ so $\Delta G^\ominus < 0$ (spontaneous).

Non-spontaneous reaction



For a non-spontaneous reaction, the equilibrium position lies further towards pure reactants meaning that at equilibrium $[\text{reactants}] > [\text{products}]$ and $K < 1$. $G^\ominus(\text{products}) > G^\ominus(\text{reactants})$ so $\Delta G^\ominus > 0$ (non-spontaneous).

ΔG , Q versus K and direction of reaction

- If a system is not at equilibrium, ΔG and Q can be used to tell us in which direction the reaction will proceed to reach equilibrium.
- For a spontaneous reaction, ΔG is negative, $Q < K$ and the reaction will proceed in the forward direction until equilibrium is reached.
- For a non-spontaneous reaction, ΔG is positive, $Q > K$ and the reaction will proceed in the reverse direction until equilibrium is reached.

Summary:

	ΔG	Q versus K	Direction of reaction
Spontaneous reaction	$\Delta G < 0$	$Q < K$	Reaction proceeds to right
Non-spontaneous reaction	$\Delta G > 0$	$Q > K$	Reaction proceeds to left
Reaction at equilibrium	$\Delta G = 0$	$Q = K$	No net change

Relationship between ΔG^\ominus and K

- The relationship between ΔG^\ominus and K is given by the following equation which can be found in section one of the IB chemistry data booklet.
- In this equation, temperature is in kelvin and ΔG^\ominus in J mol^{-1} .
- R is the universal gas constant, $8.31 \text{ J K}^{-1} \text{ mol}^{-1}$.

$$\Delta G^\ominus = -RT \ln K$$

- This equation can be rearranged to solve for K .

$$K = e^{-\frac{\Delta G}{RT}}$$

Exercises:

- 1) Calculate the value of K at 298 K for a reaction given that $\Delta G^\ominus = -33.0 \text{ kJ mol}^{-1}$

$$K = e^{-(-32960 \div (8.31 \times 298))}$$

$$K = e^{13.3}$$

$$K = 5.98 \times 10^5$$

- 2) Calculate the ΔG^\ominus for a reaction given that the K is 45.6 at 298 K.

$$\Delta G^\ominus = -8.31 \times 298 \times \ln(45.6)$$

$$\Delta G^\ominus = -9.46 \text{ kJ mol}^{-1}$$