

How far? The extent of chemical change

International Baccalaureate · IB Diploma · Chemistry · HL

Scope and prerequisites

This handout teaches Reactivity 2.3, How far? The extent of chemical change, for the course first assessed in 2025. Sections marked **AHL** are for Higher Level only.

Prerequisites: concentration in mol dm^{-3} from Structure 1.4, exothermic and endothermic reactions from Reactivity 1.1, and rates and catalysts from Reactivity 2.2. At Higher Level you will also use Gibbs energy from Reactivity 1.4 and natural logarithms.

Dynamic equilibrium

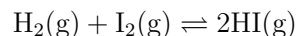
■ Why does a sealed bottle of cola stay fizzy?

In a closed bottle, carbon dioxide gas sits above the drink. Molecules of CO_2 leave the liquid and others dissolve back into it, all the time. The two rates are equal, so the amount of gas in the drink does not change and the drink stays fizzy for months. Open the bottle and the gas escapes: the balance is gone, and the drink goes flat.

Many chemical reactions behave the same way. They do not go to completion; they stop at a mixture of reactants and products.

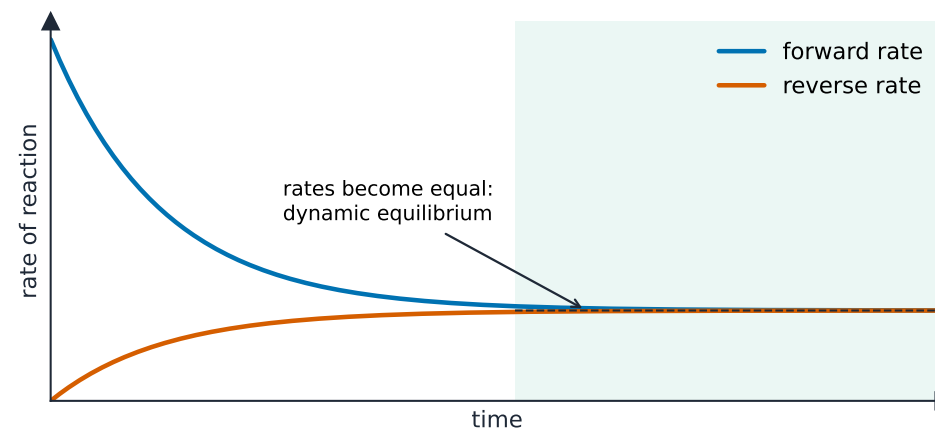
■ Reversible reactions

A **reversible reaction** can go in both directions. The sign $\rightleftharpoons$ shows this.



- The **forward reaction** goes from left to right; the **reverse reaction** goes from right to left.
- At the start only the forward reaction happens. As soon as some HI forms, the reverse reaction starts too.

■ What dynamic equilibrium means



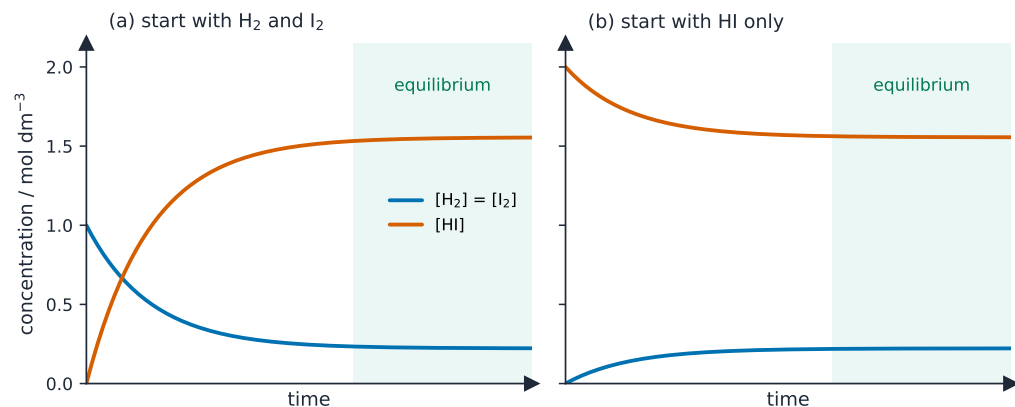
$$\text{at equilibrium: rate}_f = \text{rate}_r \cdot K_c = \frac{[\text{products}]}{[\text{reactants}]}$$

At equilibrium the two rates are equal, but neither is zero

A **dynamic equilibrium** is reached in a **closed system** when the rate of the forward reaction equals the rate of the reverse reaction.

- **Dynamic:** both reactions keep going. Particles still react, but the forward and reverse changes cancel.
- **Constant concentrations:** the amounts of reactants and products no longer change.
- **Not equal concentrations:** “constant” does not mean “the same”. At equilibrium a mixture can be mostly products or mostly reactants.
- **Closed system:** nothing enters or leaves. If a product escapes, as CO_2 escapes from an open bottle, equilibrium is never reached.

■ The same equilibrium from both sides



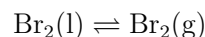
Under the same conditions you reach the same equilibrium mixture from either direction

At 700 K, 1.00 mol dm^{-3} each of H_2 and I_2 reacts until $[\text{HI}] = 1.56 \text{ mol dm}^{-3}$ and $[\text{H}_2] = [\text{I}_2] = 0.22 \text{ mol dm}^{-3}$. Starting with 2.00 mol dm^{-3} of HI alone gives the same final mixture.

Evidence that equilibrium is dynamic. Add a little D_2 (hydrogen-2, a heavier isotope of hydrogen) to an equilibrium mixture of H_2 , I_2 and HI. The concentrations do not change, but soon DI appears in the mixture. Molecules are still reacting in both directions.

Physical equilibria

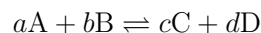
Equilibrium is not only for reactions. In a closed flask of bromine, liquid evaporates and vapour condenses at equal rates, so the brown colour of the vapour stays constant:



The equilibrium constant

The equilibrium law

For the general reaction



the **equilibrium constant** K_c is

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

- Square brackets mean concentration in mol dm^{-3} **at equilibrium**.
- Products go on top, reactants underneath.

- Each concentration is raised to the power of its coefficient in the balanced equation.
- For a given reaction, K_c has the same value at a given temperature, whatever the starting amounts. It changes only when the temperature changes.

Worked example: calculating K_c

At 700 K the equilibrium mixture for $\text{H}_2 + \text{I}_2 \rightleftharpoons 2\text{HI}$ contains $[\text{H}_2] = [\text{I}_2] = 0.020 \text{ mol dm}^{-3}$ and $[\text{HI}] = 0.14 \text{ mol dm}^{-3}$.

$$K_c = \frac{[\text{HI}]^2}{[\text{H}_2][\text{I}_2]} = \frac{0.14^2}{0.020 \times 0.020} = \frac{0.0196}{0.00040} = 49$$

IB questions usually give and expect K_c as a number, without units.

Writing K_c for other equations

Equation	K_c
$\text{N}_2 + 3\text{H}_2 \rightleftharpoons 2\text{NH}_3$	$\frac{[\text{NH}_3]^2}{[\text{N}_2][\text{H}_2]^3}$
$2\text{SO}_2 + \text{O}_2 \rightleftharpoons 2\text{SO}_3$	$\frac{[\text{SO}_3]^2}{[\text{SO}_2]^2[\text{O}_2]}$
$2\text{HI} \rightleftharpoons \text{H}_2 + \text{I}_2$ (reverse of the example)	$\frac{[\text{H}_2][\text{I}_2]}{[\text{HI}]^2} = \frac{1}{49} = 0.020$

- Reversing an equation gives $1/K_c$.
- Doubling every coefficient squares K_c : for $2\text{H}_2 + 2\text{I}_2 \rightleftharpoons 4\text{HI}$, $K_c = 49^2 = 2401$.

What the size of K tells you

The **position of equilibrium** says whether the mixture is mainly reactants or mainly products.

Value of K	Equilibrium mixture	Example
$K \gg 1$ (say 10^{10})	almost all products; the reaction "goes to completion"	burning methane
$K \approx 1$	similar amounts of reactants and products	ester formation, $K_c \approx 4$
$K \ll 1$ (say 10^{-10})	almost all reactants; hardly any reaction	$\text{N}_2 + \text{O}_2 \rightarrow 2\text{NO}$ at room temperature

K tells you **how far** a reaction goes, not **how fast**. A reaction with a huge K can still be very slow, for example the burning of a diamond at room temperature.

Le Chatelier's principle

■ The principle

Le Chatelier's principle : when a system at equilibrium is disturbed, the position of equilibrium shifts to reduce the effect of the change.

To predict a shift, first write the balanced equation with state symbols and the sign of ΔH for the forward reaction.

■ Changing a concentration

Add more of a reactant: the system uses some of it up, so the equilibrium shifts to the right and more product forms. Remove a product: the system makes more of it, again a shift to the right.

K_c does **not** change. The concentrations rearrange until the fraction in the K_c expression has its old value again.

■ Changing the pressure

Pressure matters only for gases. Count the moles of gas on each side.

- Increase the pressure: the equilibrium shifts to the side with **fewer** gas molecules, which lowers the pressure.
- Decrease the pressure: the equilibrium shifts to the side with **more** gas molecules.
- Same number on both sides, as in $\text{H}_2 + \text{I}_2 \rightleftharpoons 2\text{HI}$ (2 and 2): pressure has no effect on the position.

For $\text{N}_2(\text{g}) + 3\text{H}_2(\text{g}) \rightleftharpoons 2\text{NH}_3(\text{g})$ there are 4 gas molecules on the left and 2 on the right, so a higher pressure shifts the equilibrium to the right and gives more ammonia.

■ Changing the temperature

Temperature is the only change that alters the value of K .

- Raise the temperature: the equilibrium shifts in the **endothermic** direction, which takes in heat.
- Lower the temperature: it shifts in the **exothermic** direction.



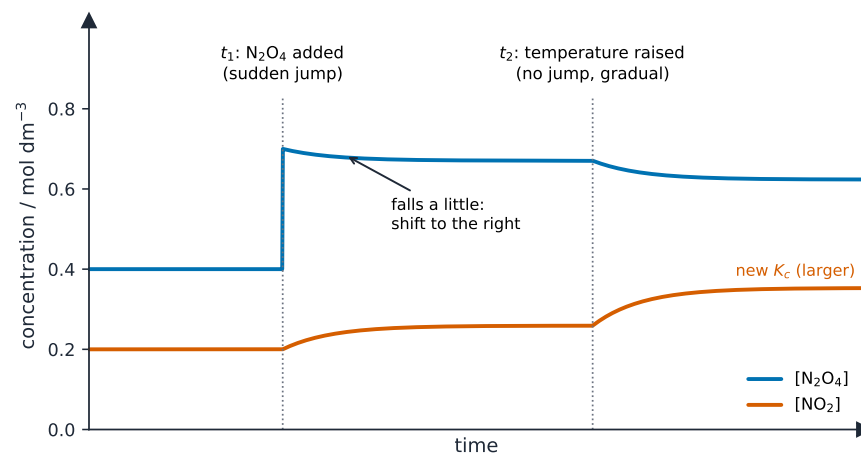
N_2O_4 is colourless and NO_2 is brown. The forward reaction is endothermic, so heating the gas shifts the equilibrium to the right: the gas turns darker brown and K_c becomes larger. In ice water the gas turns pale.

For an exothermic forward reaction the opposite is true: a higher temperature gives a smaller K and less product.

■ Adding a catalyst

A catalyst speeds up the forward and reverse reactions by the same factor. Equilibrium is reached sooner, but the position of equilibrium and K do not change.

■ Summary

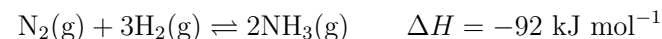


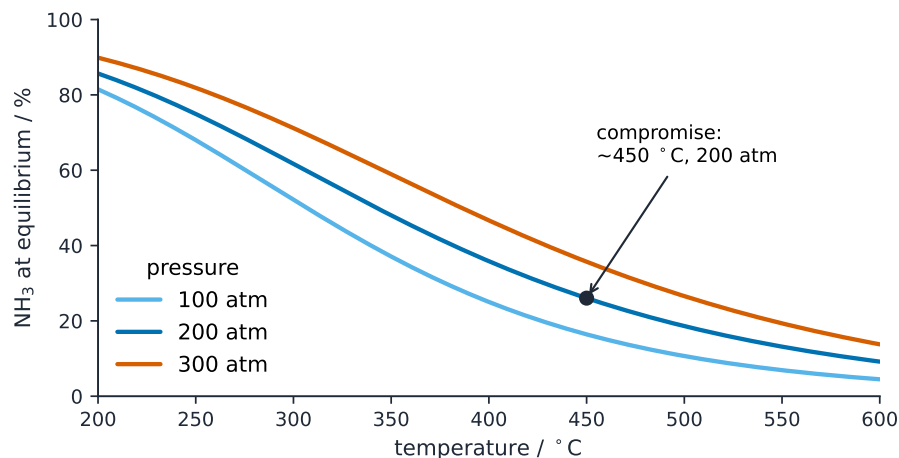
A concentration change gives a sudden jump; a temperature change gives smooth curves and a new K_c

Change	Shift in position	Effect on K
add a reactant or remove a product	to the right	none
increase the pressure (gases)	to the side with fewer gas molecules	none
raise the temperature	in the endothermic direction	changes
add a catalyst	none; equilibrium is reached sooner	none

■ Industry: making ammonia

The Haber process makes ammonia for fertilizers:





exothermic: lower $T \uparrow$ yield · higher $P \uparrow$ yield

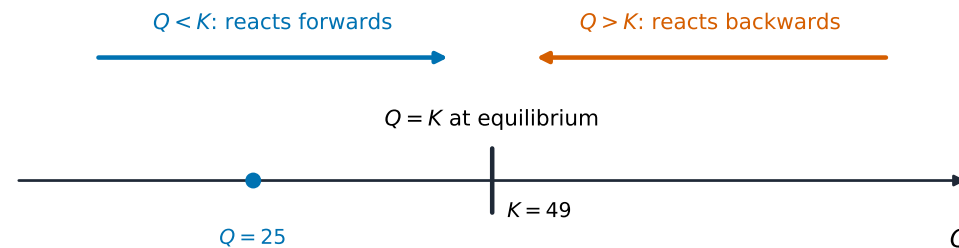
The equilibrium yield is highest at low temperature and high pressure

- **Pressure about 200 atm.** Fewer gas molecules on the right, so high pressure gives a higher **yield**. Even higher pressure would cost too much in equipment and energy.
- **Temperature about 450°C .** The forward reaction is exothermic, so a low temperature gives a higher yield, but the reaction would be far too slow. 450°C is a **compromise** between yield and rate.
- **Iron catalyst.** It makes the reaction faster; it does not change the yield.
- **Ammonia is removed** by cooling it to a liquid, and unreacted N_2 and H_2 are recycled. Removing the product keeps shifting the equilibrium to the right.

AHL: The reaction quotient

■ Q for a mixture that is not at equilibrium

The **reaction quotient** Q has the same expression as K , but uses the concentrations at any moment, not only at equilibrium.



Compare Q with K to see which way the mixture will react

- $Q < K$: too little product. The forward reaction goes faster until $Q = K$.
- $Q > K$: too much product. The reverse reaction goes faster until $Q = K$.
- $Q = K$: the mixture is already at equilibrium.

■ Worked example: which way?

At 700 K, $K_c = 49$ for $\text{H}_2 + \text{I}_2 \rightleftharpoons 2\text{HI}$. A flask contains $[\text{H}_2] = [\text{I}_2] = 0.10 \text{ mol dm}^{-3}$ and $[\text{HI}] = 0.50 \text{ mol dm}^{-3}$.

$$Q = \frac{0.50^2}{0.10 \times 0.10} = \frac{0.25}{0.010} = 25$$

Q (25) is less than K (49), so the mixture is not at equilibrium. It reacts forwards: $[\text{HI}]$ rises and $[\text{H}_2]$ and $[\text{I}_2]$ fall until Q reaches 49.

AHL: Equilibrium calculations

■ The ICE table

To find equilibrium amounts, set out three rows:

- Initial amounts.
- Change, in the mole ratio of the equation.
- Equilibrium amounts = initial + change.

■ Worked example: finding K_c

1.00 mol of ethanoic acid and 1.00 mol of ethanol are heated with a little acid catalyst until equilibrium. The mixture then contains 0.67 mol of ethyl ethanoate.

	CH_3COOH	$\text{C}_2\text{H}_5\text{OH}$	$\text{CH}_3\text{COOC}_2\text{H}_5$	H_2O
Initial / mol	1.00	1.00	0	0
Change / mol	-0.67	-0.67	+0.67	+0.67
Equilibrium / mol	0.33	0.33	0.67	0.67

The volume V is the same for every substance, and there are 2 particles on each side, so V cancels:

$$K_c = \frac{(0.67/V)(0.67/V)}{(0.33/V)(0.33/V)} = \frac{0.67^2}{0.33^2} = 4.1$$

■ **Worked example: finding equilibrium concentrations**

At 700 K, $K_c = 49$ for $\text{H}_2 + \text{I}_2 \rightleftharpoons 2\text{HI}$. Start with 1.00 mol dm^{-3} each of H_2 and I_2 and no HI . Let $x \text{ mol dm}^{-3}$ of H_2 react.

	H_2	I_2	HI
Initial	1.00	1.00	0
Change	$-x$	$-x$	$+2x$
Equilibrium	$1.00 - x$	$1.00 - x$	$2x$

$$49 = \frac{(2x)^2}{(1.00 - x)^2}$$

Both sides are perfect squares, so take the square root:

$$7.0 = \frac{2x}{1.00 - x} \Rightarrow 7.0 - 7.0x = 2x \Rightarrow x = 0.78$$

So $[\text{HI}] = 1.56 \text{ mol dm}^{-3}$ and $[\text{H}_2] = [\text{I}_2] = 0.22 \text{ mol dm}^{-3}$. These are the values in the concentration–time graphs above.

■ **When K is very small**

If K is very small, very little reactant is used up. You may then take the equilibrium concentration of each reactant as equal to its initial concentration. This **approximation** avoids solving a quadratic.

At a high temperature, $K_c = 4.0 \times 10^{-4}$ for $\text{N}_2(\text{g}) + \text{O}_2(\text{g}) \rightleftharpoons 2\text{NO}(\text{g})$. Start with $[\text{N}_2] = [\text{O}_2] = 0.50 \text{ mol dm}^{-3}$.

$$K_c = \frac{[\text{NO}]^2}{[\text{N}_2][\text{O}_2]} \approx \frac{[\text{NO}]^2}{0.50 \times 0.50} = 4.0 \times 10^{-4}$$

$$[\text{NO}]^2 = 1.0 \times 10^{-4} \Rightarrow [\text{NO}] = 0.010 \text{ mol dm}^{-3}$$

Only $0.005 \text{ mol dm}^{-3}$ of N_2 was used, 1% of 0.50, so the approximation was fair. State the assumption in your answer.

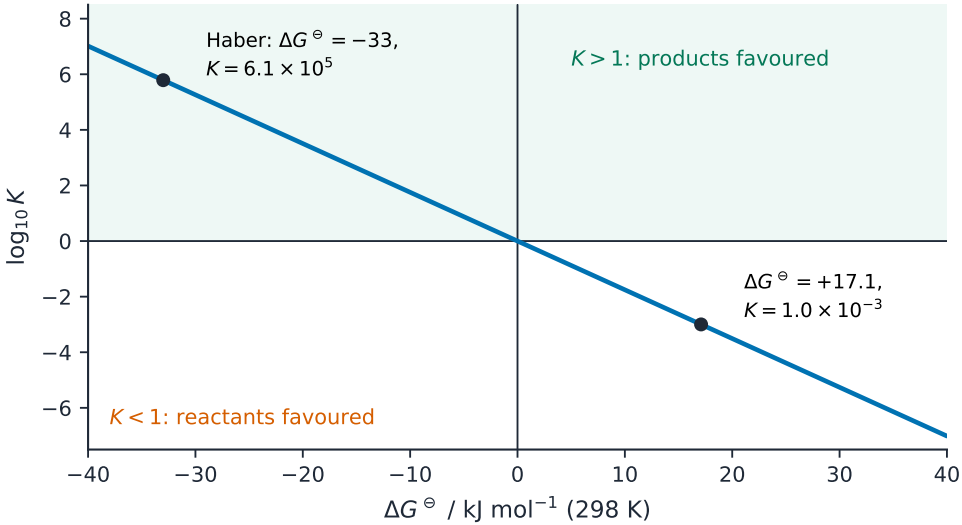
AHL: Equilibrium and Gibbs energy

■ **Linking $\Delta G^\ominus$ and K**

The standard **Gibbs energy** change of a reaction and its equilibrium constant are linked (data booklet):

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

$$R = 8.31 \text{ J K}^{-1} \text{ mol}^{-1}, T \text{ in K}, \Delta G^\ominus \text{ in J mol}^{-1}.$$



A negative $\Delta G^\ominus$ means $K > 1$; a positive $\Delta G^\ominus$ means $K < 1$

$\Delta G^\ominus$	K	Equilibrium mixture
negative	greater than 1	mainly products
zero	1	similar amounts
positive	less than 1	mainly reactants

At equilibrium the mixture has the lowest Gibbs energy it can reach, so $\Delta G = 0$ for any further change. A reaction with a positive $\Delta G^\ominus$ still happens a little: it reaches an equilibrium that lies to the left.

■ **Worked example:** K from $\Delta G^\ominus$

For the Haber process, $\Delta G^\ominus = -33 \text{ kJ mol}^{-1}$ at 298 K.

$$\ln K = \frac{-\Delta G^\ominus}{RT} = \frac{33\,000}{8.31 \times 298} = 13.3 \quad \Rightarrow \quad K = e^{13.3} = 6.1 \times 10^5$$

At room temperature the equilibrium lies far to the right. Industry still heats the gases, because at 298 K the reaction is far too slow.

■ **Worked example:** $\Delta G^\ominus$ from K

A reaction has $K = 1.0 \times 10^{-3}$ at 298 K.

$$\Delta G^\ominus = -8.31 \times 298 \times \ln(1.0 \times 10^{-3}) = -2476 \times (-6.91) = +17\,100 \text{ J mol}^{-1} = +17.1 \text{ kJ mol}^{-1}$$

Practice

- State two features of a dynamic equilibrium.
- Explain why a mixture of calcium carbonate and its decomposition products in an open container never reaches equilibrium.
- Write the K_c expression for $4\text{NH}_3(\text{g}) + 5\text{O}_2(\text{g}) \rightleftharpoons 4\text{NO}(\text{g}) + 6\text{H}_2\text{O}(\text{g})$.
- For $\text{PCl}_5 \rightleftharpoons \text{PCl}_3 + \text{Cl}_2$, the equilibrium concentrations are $[\text{PCl}_5] = 0.040$, $[\text{PCl}_3] = 0.020$ and $[\text{Cl}_2] = 0.080 \text{ mol dm}^{-3}$. Calculate K_c .
- $K_c = 2.5 \times 10^{-31}$ for a reaction at 298 K. Describe the equilibrium mixture.
- $\text{CO}(\text{g}) + 2\text{H}_2(\text{g}) \rightleftharpoons \text{CH}_3\text{OH}(\text{g})$, $\Delta H = -91 \text{ kJ mol}^{-1}$. Predict the effect on the yield of methanol of (a) raising the pressure, (b) raising the temperature, (c) adding a catalyst.
- A sealed syringe of N_2O_4 and NO_2 is put into hot water. State and explain the colour change.
- Explain why the Haber process runs at about 450°C and not at room temperature.
- AHL.** For $\text{H}_2 + \text{I}_2 \rightleftharpoons 2\text{HI}$, $K_c = 49$. A mixture has $[\text{H}_2] = [\text{I}_2] = 0.050$ and $[\text{HI}] = 0.60 \text{ mol dm}^{-3}$. Calculate Q and state the direction of change.
- AHL.** 2.00 mol of SO_2 and 1.00 mol of O_2 are mixed in a 1.00 dm^3 flask. At equilibrium, 1.60 mol of SO_3 is present. Calculate K_c for $2\text{SO}_2 + \text{O}_2 \rightleftharpoons 2\text{SO}_3$.
- AHL.** $K_c = 4.0$ for $\text{CH}_3\text{COOH} + \text{C}_2\text{H}_5\text{OH} \rightleftharpoons \text{CH}_3\text{COOC}_2\text{H}_5 + \text{H}_2\text{O}$. Starting with 1.00 mol of acid and 1.00 mol of ethanol, calculate the amount of ester at equilibrium.
- AHL.** For $\text{A}(\text{g}) \rightleftharpoons 2\text{B}(\text{g})$, $K_c = 1.6 \times 10^{-5}$. The initial $[\text{A}]$ is 0.10 mol dm^{-3} . Use an approximation to find $[\text{B}]$ at equilibrium, and state the assumption.
- AHL.** Calculate K at 298 K for a reaction with $\Delta G^\ominus = -11.4 \text{ kJ mol}^{-1}$.

Answers.

- The forward and reverse rates are equal; the concentrations stay constant (both reactions still happen). It needs a closed system.
- CO_2 gas escapes, so the reverse reaction $\text{CaO} + \text{CO}_2 \rightarrow \text{CaCO}_3$ cannot keep pace. The system is not closed.
- $K_c = \frac{[\text{NO}]^4[\text{H}_2\text{O}]^6}{[\text{NH}_3]^4[\text{O}_2]^5}$
- $K_c = \frac{0.020 \times 0.080}{0.040} = 0.040$.
- K_c is extremely small, so the mixture is almost all reactants; hardly any product forms.
- (a) Yield increases: 3 gas molecules on the left, 1 on the right, so the equilibrium shifts to the right. (b) Yield decreases: the forward reaction is exothermic, so the equilibrium shifts left (endothermic direction) and K falls. (c) No change in yield; equilibrium is reached faster.
- It turns darker brown. The forward reaction $\text{N}_2\text{O}_4 \rightarrow 2\text{NO}_2$ is endothermic, so a higher temperature shifts the equilibrium to the right, making more brown NO_2 .
- A lower temperature would give a higher equilibrium yield (exothermic forward reaction) but the rate would be too slow. 450°C gives a reasonable yield at a reasonable rate: a compromise.
- AHL.** $Q = 0.60^2/(0.050 \times 0.050) = 0.36/0.0025 = 144$. $Q > K$, so the mixture reacts backwards: $[\text{HI}]$ falls, $[\text{H}_2]$ and $[\text{I}_2]$ rise.
- AHL.** Change: $\text{SO}_3 +1.60$, $\text{SO}_2 -1.60$, $\text{O}_2 -0.80$. Equilibrium: SO_2 0.40, O_2 0.20, SO_3 1.60 mol dm^{-3} . $K_c = 1.60^2/(0.40^2 \times 0.20) = 2.56/0.032 = 80$.
- AHL.** $4.0 = x^2/(1.00 - x)^2$, so $2.0 = x/(1.00 - x)$, $x = 2.0 - 2.0x$, $x = 0.67 \text{ mol}$ of ester.
- AHL.** Assume $[\text{A}]$ stays 0.10. $[\text{B}]^2 = 1.6 \times 10^{-5} \times 0.10 = 1.6 \times 10^{-6}$, $[\text{B}] = 1.3 \times 10^{-3} \text{ mol dm}^{-3}$. Assumption: so little A reacts ($6 \times 10^{-4} \text{ mol dm}^{-3}$, under 1%) that $[\text{A}]$ at equilibrium equals its initial value.
- AHL.** $\ln K = 11\,400/(8.31 \times 298) = 4.60$; $K = e^{4.60} = 99$, or 1.0×10^2 to 2 significant figures.

Exam tips

- “Dynamic” means both reactions continue; “equilibrium” means the rates are equal. Never write that the concentrations are equal.
- Write K_c with products over reactants and coefficients as powers; use equilibrium concentrations only.
- Only temperature changes K . Concentration and pressure change the position; a catalyst changes neither.
- For a temperature question, state the sign of ΔH first; for a pressure question, count the gas molecules on each side.

- **AHL.** Compare Q with K before saying which way a mixture reacts.
- **AHL.** In an ICE table the changes follow the mole ratio; convert moles to concentrations unless the volume cancels.
- **AHL.** In $\Delta G^\ominus = -RT \ln K$, convert kJ to J.