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Reactivity 2.3 HL
The Reaction Quotient, Equilibrium Calculations and Gibbs Energy

Booklet 6 · Understandings 2.3.5 – 2.3.7

Predicting the direction of a reaction with Q, using ICE tables to find K and equilibrium concentrations, the small-K approximation, and how $\Delta G^{\ominus}$ and K both measure the position of equilibrium

Complete revision notes, 16 worked examples, model answers & 36 practice questions · Higher Level

How the level tags work in this booklet

HL Everything in this booklet is HL-only content. It builds directly on Booklet 5 (Reactivity 2.3.1–2.3.4: dynamic equilibrium, the equilibrium law, *K* and Le Chatelier's principle), which is assumed throughout.

★ marks harder, multi-step examples and questions.

Inside this booklet

1. What the syllabus actually asks of you
2. 2.3.5 — The reaction quotient, *Q*
3. 2.3.6 — Finding *K* with ICE tables
4. 2.3.6 — Finding equilibrium concentrations
5. 2.3.6 — When *K* is very small
6. 2.3.7 — Gibbs energy and *K*
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8. Check yourself
9. Answers

1 What the syllabus actually asks of you

Booklet 5 treated equilibrium qualitatively: what K means and which way an equilibrium shifts. This HL booklet makes it quantitative. The reaction quotient, Q, tells you which way a mixture that is not yet at equilibrium will react. The equilibrium law, set out in an ICE table, lets you calculate K from experimental data, or the equilibrium concentrations from K. Finally, the standard Gibbs energy change links equilibrium to the thermodynamics of Reactivity 1.4: $\Delta G^{\ominus}$ and K are two ways of measuring the same thing. Expect these calculations in Paper 1B and Paper 2, often in several linked parts, and expect them again in Reactivity 3.1 for weak acids and bases.

Understanding	What it says	What you must be able to do	Level
2.3.5 Reaction quotient	The reaction quotient, Q, is calculated using the equilibrium expression with non-equilibrium concentrations of reactants and products.	Calculate 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.	HL
2.3.6 Equilibrium calculations	The equilibrium law is the basis for quantifying the composition of an equilibrium mixture.	Solve problems involving values of K and initial and equilibrium concentrations of the components of an equilibrium mixture. **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.**	HL
2.3.7 Gibbs energy	The equilibrium constant and Gibbs energy change, ΔG, can both be used to measure the position of an equilibrium reaction.	Calculations using the equation $\Delta G^{\ominus} = -RT \ln K$. The equation is given in the data booklet.	HL

Linking questions and connections for 2.3.5 – 2.3.7

- **Reactivity 3.1:** how does the equilibrium law help us to determine the pH of a weak acid, weak base or a buffer solution? → section 5.2
- **Reactivity 1.4:** how can Gibbs energy be used to explain which of the forward or backward reaction is favoured before reaching equilibrium? → section 6.1
- **Reactivity 2.2:** for a single-step reaction, K is the ratio of the forward and backward rate constants, k/k' → section 6.4
- **Booklet 5:** Q explains Le Chatelier's principle: a change in concentration or pressure changes Q, and the system reacts until $Q = K$ again → section 2.3

What the data booklet does and does not give you

It gives you: $\Delta G^{\ominus} = -RT \ln K$; $\Delta G^{\ominus} = \Delta H^{\ominus} - T\Delta S^{\ominus}$; and $R = 8.31\ \text{J K}^{-1}\ \text{mol}^{-1}$.

It does not give you: the meaning of Q or the rules comparing Q with K; the ICE-table method; the small-K approximation; or the need to convert kJ to J. All of these must be learned.

2 Reactivity 2.3.5 — The reaction quotient, Q

HL

2.1 What Q is

The equilibrium constant expression only gives K when you substitute **equilibrium** concentrations. If you substitute the concentrations at any other moment, the number you get is the reaction quotient, Q. As the reaction proceeds, the concentrations change and Q changes with them, always moving towards K. When Q reaches K, the mixture is at equilibrium and stops changing.

Definition to learn

The **reaction quotient**, Q, is the value obtained by substituting the concentrations of reactants and products, all measured at the same time, into the equilibrium constant expression. For $aA + bB \rightleftharpoons cC + dD$:

$$Q = [C]^c[D]^d / [A]^a[B]^b \quad \text{(any concentrations)}$$

K has one fixed value at a given temperature; Q can have any value.

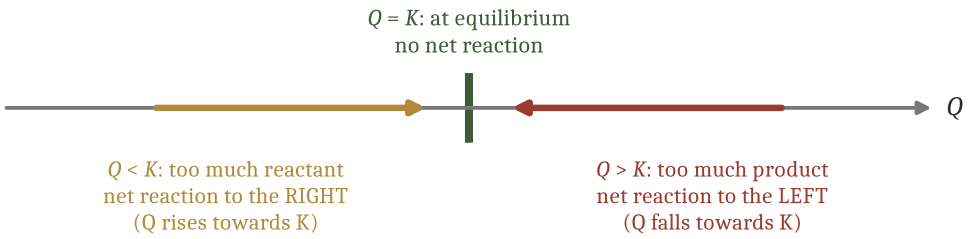


Figure 1 — Comparing Q with K tells you the direction of net reaction.

Comparison	What it means	Direction of net reaction
$Q = K$	the mixture is at equilibrium	no net reaction
$Q < K$	too much reactant, too little product	to the **right**, towards products
$Q > K$	too much product, too little reactant	to the **left**, towards reactants

Worked example 1 — which way will each mixture react?

Q. For $H_2(g) + I_2(g) \rightleftharpoons 2HI(g)$, $K = 46.0$ at 440 °C. For each mixture (mol dm^{-3}), state whether it is at equilibrium and, if not, the direction of net reaction.

Mixture	$[H_2]$	$[I_2]$	[HI]	$Q = [HI]^2 / [H_2][I_2]$	Conclusion
1	0.0200	0.0150	0.0800	21.3	$Q < K$: goes **right**
2	0.00400	0.00500	0.0400	80.0	$Q > K$: goes **left**
3	0.0100	0.0100	0.0678	46.0	$Q = K$: at equilibrium

In mixture 1, HI forms until Q rises to 46.0; in mixture 2, HI decomposes until Q falls to 46.0 (Figure 2).

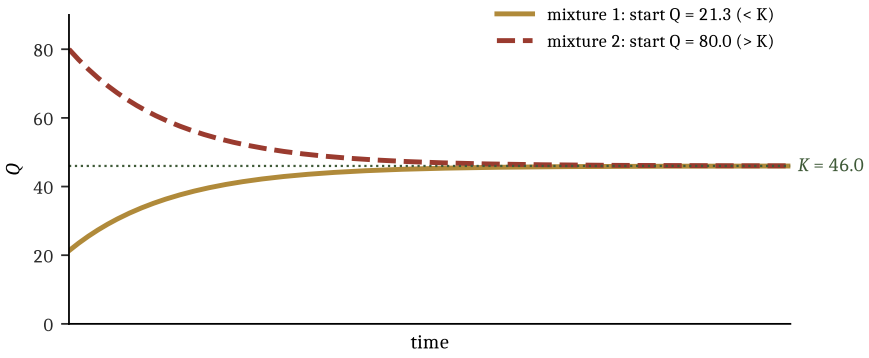


Figure 2 — Mixtures 1 and 2 from worked example 1. Whatever its starting value, Q changes until it equals K.

Worked example 2 — Q when the coefficients are not 1

Q. For $N_2(g) + 3H_2(g) \rightleftharpoons 2NH_3(g)$, $K = 0.105$ at a certain temperature. A mixture contains $[N_2] = 0.400$, $[H_2] = 0.200$ and $[NH_3] = 0.0500$ mol dm^{-3}. Is it at equilibrium? If not, which way will it react?

$Q = [NH_3]^2 / [N_2][H_2]^3 = (0.0500)^2 / (0.400 \times 0.200^3) = 2.50 \times 10^{-3} / 3.20 \times 10^{-3} =$ **0.781**

$Q > K$ (0.781 > 0.105): **not at equilibrium; net reaction to the left**, so NH_3 decomposes until Q falls to 0.105

2.3 Q explains Le Chatelier's principle

Le Chatelier's principle predicts what happens, but not why. Q gives the reason. Adding a reactant to an equilibrium mixture makes the denominator larger, so Q falls below K and the system reacts to the right until $Q = K$ again. Changing the volume of a gas mixture changes every concentration by the same factor, so Q changes only if the numbers of gas molecules on the two sides differ. A temperature change is different: it leaves Q unchanged but changes K, and the system reacts until Q reaches the new K.

Worked example 3 — using Q to explain the effect of pressure ★

Q. For $N_2O_4(g) \rightleftharpoons 2NO_2(g)$, $K = 0.0100$. An equilibrium mixture has $[N_2O_4] = 0.0500$ and $[NO_2] = 0.0224$ mol dm^{-3}. The volume is suddenly halved. Use Q to predict the direction of the shift.

halving the volume doubles every concentration: $[N_2O_4] = 0.100$, $[NO_2] = 0.0448$ mol dm^{-3}

$Q = (0.0448)^2 / 0.100 =$ **0.0200**, twice K

$Q > K$, so **net reaction to the left**, towards the side with fewer gas molecules, as Le Chatelier predicts

In general, if every concentration is multiplied by n, Q is multiplied by $n^{\Delta n}$, where Δn is the change in the number of gas molecules. When $\Delta n = 0$, Q does not change, so pressure has no effect.

Examiner traps with Q

- Getting the direction backwards. $Q < K$ means the reaction goes forward, to make more product.
- Writing that K changes to match Q. K is fixed at a given temperature; Q moves towards K.
- Forgetting the powers when calculating Q. It uses exactly the same expression as K.
- Comparing Q with a value of K for a different temperature.

3 Reactivity 2.3.6 — Finding K with ICE tables HL

3.1 K from equilibrium concentrations

If all the equilibrium concentrations are known, substitute them into the expression, as in Booklet 5.

Worked example 4 — K from equilibrium concentrations

Q. At a certain temperature an equilibrium mixture for $CO(g) + H_2O(g) \rightleftharpoons CO_2(g) + H_2(g)$ contains $[CO] = 0.0300$, $[H_2O] = 0.0600$ and $[CO_2] = [H_2] = 0.0450$ mol dm^{-3}. Calculate K.

$K = [CO_2][H_2] / [CO][H_2O] = (0.0450 \times 0.0450) / (0.0300 \times 0.0600) = 2.025 \times 10^{-3} / 1.80 \times 10^{-3} =$ **1.13**

3.2 The ICE table

Usually you are told the starting amounts and only **one** equilibrium amount. The others must be worked out from the stoichiometry. An ICE table keeps the working organized.

Method — the ICE table

1. Write the balanced equation. Convert all amounts to concentrations (divide moles by the volume in dm^3).
2. Under the equation, write three rows: **I**nitial, **C**hange and **E**quilibrium. Initial product concentrations are zero unless you are told otherwise.
3. Find the change for the one species you know about (equilibrium − initial). Reactants decrease (−); products increase (+).
4. Use the **coefficients** to find the changes for every other species. The changes are in the mole ratio of the equation; the equilibrium concentrations are not.
5. Equilibrium = initial + change. Write the K expression, then substitute **only** the equilibrium row.

Worked example 5 — a 1 : 1 : 1 reaction in a 1.00 dm^3 flask

Q. 0.300 mol of PCl_3 and 0.200 mol of Cl_2 were placed in a 1.00 dm^3 flask and allowed to reach equilibrium: $PCl_3(g) + Cl_2(g) \rightleftharpoons PCl_5(g)$. The equilibrium mixture contained 0.180 mol of PCl_3. Calculate K.

/ mol dm^{-3}	PCl_3	Cl_2	PCl_5
Initial	0.300	0.200	0
Change	−0.120	−0.120	+0.120
Equilibrium	0.180	0.080	0.120

change in $PCl_3 = 0.180 - 0.300 = -0.120$; the 1 : 1 : 1 ratio gives the other changes

$K = [PCl_5] / [PCl_3][Cl_2] = 0.120 / (0.180 \times 0.080) =$ **8.3** (2 s.f., limited by 0.080)

Worked example 6 — a 2 : 1 : 2 reaction in a 2.00 dm^3 flask

Q. 0.400 mol SO_2 and 0.300 mol O_2 were sealed in a 2.00 dm^3 vessel. At equilibrium, 0.300 mol SO_3 had formed: $2SO_2(g) + O_2(g) \rightleftharpoons 2SO_3(g)$. Calculate K.

/ mol dm^{-3}	SO_2	O_2	SO_3
Initial	0.200	0.150	0
Change	−0.150	−0.075	+0.150
Equilibrium	0.050	0.075	0.150

divide every amount by 2.00 dm^3 first; $[SO_3]$ at equilibrium = 0.300/2.00 = 0.150

2 SO_2 and 1 O_2 are used for every 2 SO_3 formed: changes −0.150, −0.075, +0.150

$K = [SO_3]^2 / [SO_2]^2[O_2] = 0.150^2 / (0.050^2 \times 0.075) =$ **1.2×10^2**

Using moles instead of concentrations here would give K = 60, which is wrong: the volume does not cancel when the number of gas molecules changes.

Worked example 7 — when some product is present at the start ★

Q. A flask initially contained $[H_2]$ = 0.0200, $[I_2]$ = 0.0100 and [HI] = 0.0100 mol dm^{-3}. At equilibrium, $[I_2]$ = 0.00200 mol dm^{-3}. Calculate K for $H_2(g) + I_2(g) \rightleftharpoons 2HI(g)$.

/ mol dm^{-3}	H_2	I_2	HI
Initial	0.0200	0.0100	0.0100
Change	−0.0080	−0.0080	+0.0160
Equilibrium	0.0120	0.00200	0.0260

$[I_2]$ fell by 0.0080, so the net reaction went to the right; HI increases by 2 × 0.0080

$K = 0.0260^2 / (0.0120 \times 0.00200) =$ **28**

The initial HI is simply added to the change: equilibrium = initial + change for every species.

Model answer: "Explain why the equilibrium concentrations of the reactants are not in the same ratio as the coefficients in the equation, although the changes are." (2 marks)

The changes are the amounts that react, and substances always react in the mole ratio of the balanced equation [1]. The equilibrium concentrations also depend on the initial amounts chosen, which can be in any ratio, so the equilibrium concentrations are not in the stoichiometric ratio [1].

Examiner traps with ICE tables

- Using amounts in moles instead of concentrations when the volume is not 1 dm^3.
- Applying the coefficients to the equilibrium concentrations instead of to the changes.
- Substituting initial values, or the change row, into the K expression.
- Forgetting that a product present at the start still has an initial value.
- Leaving out the K expression itself. It earns a mark even if the arithmetic goes wrong.

4 Reactivity 2.3.6 — Finding equilibrium concentrations HL

4.1 One unknown concentration

Worked example 8 — one unknown equilibrium concentration

Q. For $CO(g) + 2H_2(g) \rightleftharpoons CH_3OH(g)$, $K = 14.5$ at a certain temperature. At equilibrium, $[CO] = 0.150$ and $[H_2] = 0.220$ mol dm^{-3}. Calculate $[CH_3OH]$.

$[CH_3OH] = K[CO][H_2]^2 = 14.5 \times 0.150 \times 0.220^2 =$ **0.105 mol dm^{-3}**

4.2 From K and initial concentrations: let the change be x

When you know K and the initial concentrations, let the change in one species be x, write every other change in terms of x, and solve. The syllabus does not expect quadratic equations, so exam questions are set so that the algebra simplifies, usually by taking a **square root of both sides** (when the expression is a perfect square) or by the **small-K approximation** (section 5).

Worked example 9 — a perfect square

Q. 0.0100 mol dm^{-3} each of H_2 and I_2 are heated at 440 °C, where $K = 46.0$ for $H_2(g) + I_2(g) \rightleftharpoons 2HI(g)$. Calculate the equilibrium concentrations.

/ mol dm^{-3}	H_2	I_2	HI
Initial	0.0100	0.0100	0
Change	$-x$	$-x$	$+2x$
Equilibrium	$0.0100 - x$	$0.0100 - x$	$2x$

$K = (2x)^2 / (0.0100 - x)^2 = 46.0$ → square root of both sides: $2x / (0.0100 - x) = \sqrt{46.0} = 6.782$

$2x = 0.06782 - 6.782x \rightarrow 8.782x = 0.06782 \rightarrow x = 7.72 \times 10^{-3}$

$[HI] = 2x = 0.0154$ mol dm^{-3}; $[H_2] = [I_2] = 0.0100 - 0.00772 = 0.0023$ mol dm^{-3}

Check: $0.0154^2 / 0.00228^2 = 46.0$ √. Do not stop at x: the question asks for the concentrations.

Worked example 10 — starting from the product side ★

Q. Hydrogen iodide at an initial concentration of 0.500 mol dm^{-3} decomposes: $2HI(g) \rightleftharpoons H_2(g) + I_2(g)$, $K = 0.0200$. Calculate the equilibrium concentrations.

/ mol dm^{-3}	HI	H_2	I_2
Initial	0.500	0	0
Change	$-2x$	$+x$	$+x$
Equilibrium	$0.500 - 2x$	x	x

$K = x^2 / (0.500 - 2x)^2 = 0.0200 \rightarrow x / (0.500 - 2x) = \sqrt{0.0200} = 0.1414$

$x = 0.07071 - 0.2828x \rightarrow 1.2828x = 0.07071 \rightarrow x = 0.0551$

$[H_2] = [I_2] = 0.0551$ mol dm^{-3}; $[HI] = 0.500 - 0.110 = 0.390$ mol dm^{-3}

Choosing the change in HI as $-2x$ (rather than $-x$) avoids fractions. Choose x to fit the smallest coefficient.

Examiner traps when solving for x

- Reaching for the quadratic formula. At this level there is always a square root or an approximation; if not, look for your mistake.
- Forgetting to apply the coefficients to x: 2HI changes by $2x$, and $(2x)^2 = 4x^2$, not $2x^2$.
- Stopping at x instead of calculating each equilibrium concentration.
- Not checking that the answer makes sense: no equilibrium concentration can be negative.

5 Reactivity 2.3.6 — When K is very small HL

5.1 The approximation

If K is very small (as a rule of thumb, less than about 10^{-3}), the reaction hardly proceeds, so the amount of reactant used up is tiny compared with the amount present. You can then assume:

$$[\text{reactant}]_{\text{equilibrium}} \approx [\text{reactant}]_{\text{initial}} \quad \text{that is, (initial} - x) \approx \text{initial}$$

Apply the approximation only to terms where x is **subtracted from** (or added to) a much larger number. Never drop x where it is multiplied or stands alone, as in the product terms: those small values are exactly what you are calculating. Always state the approximation and why it is justified, and check it at the end.

Worked example 11 — a gas-phase reaction with very small K

Q. At a high temperature, $2NOCl(g) \rightleftharpoons 2NO(g) + Cl_2(g)$ has $K = 1.0 \times 10^{-8}$. Calculate [NO] at equilibrium when the initial [NOCl] is 0.500 mol dm^{-3}.

/ mol dm^{-3}	NOCl	NO	Cl_2
Initial	0.500	0	0
Change	$-2x$	$+2x$	$+x$
Equilibrium	$0.500 - 2x \approx 0.500$	$2x$	x

K is very small, so $2x \ll 0.500$ and [NOCl] ≈ 0.500

$K = (2x)^2 x / (0.500)^2 = 4x^3 / 0.250 = 1.0 \times 10^{-8} \rightarrow x^3 = 6.25 \times 10^{-10} \rightarrow x = 8.55 \times 10^{-4}$

[NO] = $2x = 1.7 \times 10^{-3}$ mol dm^{-3}

check: $2x$ is 0.34 % of 0.500, so the approximation was justified

5.2 Weak acids: a preview of Reactivity 3.1

Weak acids dissociate only slightly, so their K values are small and the same approximation applies. This is how the pH of a weak acid is calculated in Reactivity 3.1.

Worked example 12 — the equilibrium in a weak acid solution

Q. For ethanoic acid, $CH_3COOH(aq) \rightleftharpoons CH_3COO^-(aq) + H^+(aq)$, $K = 1.8 \times 10^{-5}$. Calculate [H^+] in a 0.100 mol dm^{-3} solution and the percentage of the acid that dissociates.

let [H^+] = [CH_3COO^-] = x; [CH_3COOH] = $0.100 - x \approx 0.100$ (K very small)

$K = x^2 / 0.100 = 1.8 \times 10^{-5} \rightarrow x^2 = 1.8 \times 10^{-6} \rightarrow$ **[H^+] = 1.34×10^{-3} mol dm^{-3}**

percentage dissociated = $1.34 \times 10^{-3} / 0.100 \times 100$ = **1.3 %** (small, so the approximation holds)

In Reactivity 3.1 you will convert this to pH: $-\log_{10}(1.34 \times 10^{-3}) = 2.87$.

Model answer: "State the approximation used in calculating [NO], and explain why it is justified." (2 marks)

The equilibrium concentration of NOCl is assumed to equal its initial concentration ($0.500 - 2x \approx 0.500$) [1]. K is very small, so the equilibrium lies far to the left and only a negligible fraction of NOCl reacts; the calculated $2x$ is less than 1 % of 0.500 [1].

Examiner traps with the small-K approximation

- Using it when K is not small (for example $K = 4$): the answer is then badly wrong.
- Dropping x from the product terms as well, which gives zero.
- Not stating the approximation, or not justifying it from the size of K.

6 Reactivity 2.3.7 — Gibbs energy and K HL

6.1 Equilibrium is the minimum of Gibbs energy

In Reactivity 1.4, the sign of the Gibbs energy change, ΔG, showed which way a reaction is spontaneous. A negative ΔG means the forward reaction is spontaneous for the current mixture; a positive ΔG means the backward reaction is; $\Delta G = 0$ means the mixture is at equilibrium. As a reaction proceeds, the total Gibbs energy of the mixture falls, whether you start from pure reactants or pure products. So it must pass through a **minimum**, and that minimum is the equilibrium mixture. At the minimum no more work can be obtained from the system: a battery at equilibrium is flat. Because Gibbs energy is lowest, the total entropy (system plus surroundings) is at its **maximum**.

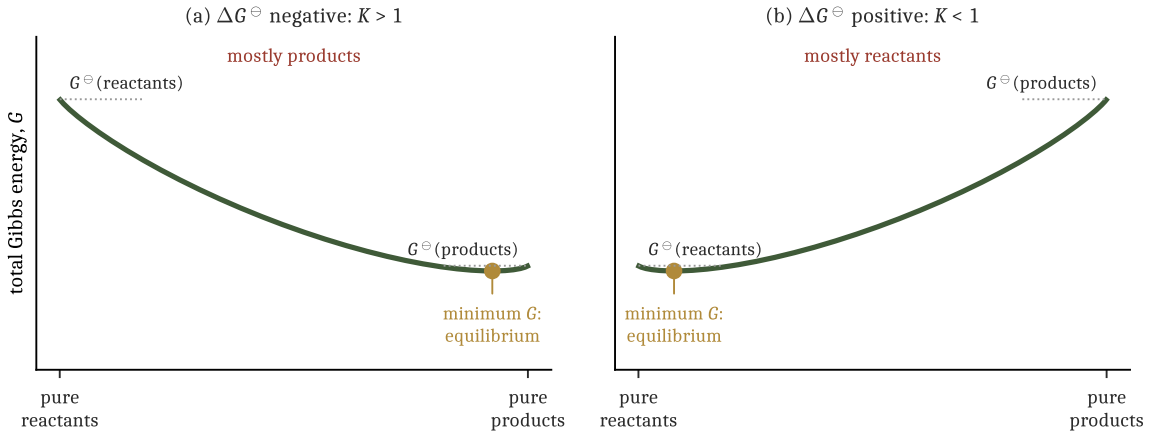


Figure 3 — Total Gibbs energy of the reaction mixture against composition. (a) When $G^\ominus$(products) < $G^\ominus$(reactants), $\Delta G^\ominus$ is negative and the minimum lies close to the products. (b) When $\Delta G^\ominus$ is positive the minimum lies close to the reactants.

6.2 The link between $\Delta G^\ominus$ and K

Equation to learn (in the data booklet)

$$\Delta G^\ominus = -RT \ln K \quad \text{so} \quad K = e^{-\Delta G^\ominus / RT}$$

$\Delta G^\ominus$ is the standard Gibbs energy change, in **J** mol^{-1}; R = 8.31 J K^{-1} mol^{-1}; T is in kelvin. $\Delta G^\ominus$ refers to the change from pure reactants to pure products in their standard states; ΔG (without $\ominus$) is the value for the actual mixture, and is zero at equilibrium.

$\Delta G^\ominus$	ln K	K	Equilibrium mixture
negative	positive	> 1	mainly products
0	0	= 1	appreciable amounts of both
positive	negative	< 1	mainly reactants

Because the relationship is logarithmic, a modest $\Delta G^\ominus$ corresponds to a huge range of K. At 298 K, every 5.7 kJ mol^{-1} changes K by a factor of 10 (Figure 4). This is why so many reactions have K either very large or very small.

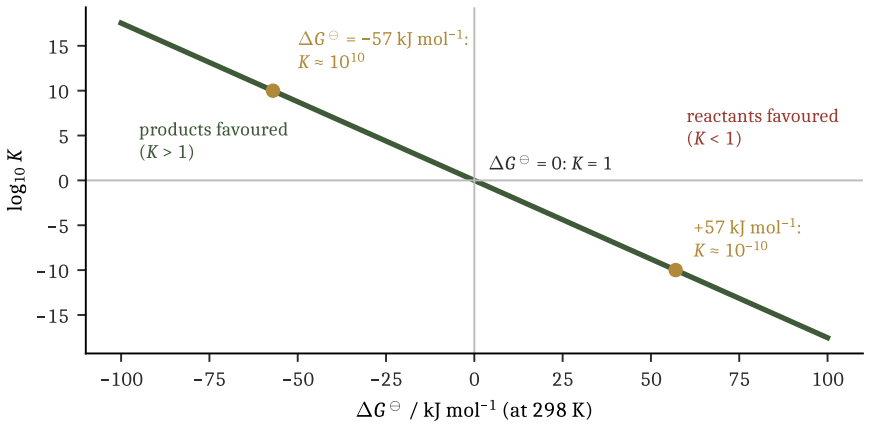


Figure 4 — $\log_{10} K$ against $\Delta G^\ominus$ at 298 K. A $\Delta G^\ominus$ of ±57 kJ mol^{-1} corresponds to $K \approx 10^{\mp 10}$.

Worked example 13 — from K to $\Delta G^\ominus$, and back

Q. (a) For $2NO(g) + O_2(g) \rightleftharpoons 2NO_2(g)$, $K = 1.7 \times 10^{12}$ at 298 K. Calculate $\Delta G^\ominus$. (b) The esterification $CH_3COOH + C_2H_5OH \rightleftharpoons CH_3COOC_2H_5 + H_2O$ has $\Delta G^\ominus = -4.38$ kJ mol^{-1} at 298 K. Calculate K.

(a) $\Delta G^\ominus = -8.31 \times 298 \times \ln(1.7 \times 10^{12}) = -2476 \times 28.16 = -6.97 \times 10^4$ J mol^{-1} = **−69.7 kJ mol^{-1}**

(b) $\ln K = -\Delta G^\ominus / RT = -(-4380) / (8.31 \times 298) = 1.769 \rightarrow K = e^{1.769} =$ **5.86**

Convert kJ to J first: using −4.38 with $R = 8.31$ gives $\ln K = 0.00177$ and $K \approx 1.00$, a meaningless answer.

Worked example 14 — predicting K for a reaction that is hard to measure

Q. Calculate K at 298 K for reactions with (a) $\Delta G^\ominus = -33.0$ kJ mol^{-1} and (b) $\Delta G^\ominus = +20.0$ kJ mol^{-1}, and describe each equilibrium mixture.

(a) $K = e^{33000/(8.31 \times 298)} = e^{13.33} =$ **6.1×10^5**: mainly products

(b) $K = e^{-20000/(8.31 \times 298)} = e^{-8.08} =$ **3.1×10^{-4}**: mainly reactants

This is useful when a reaction is too slow to reach equilibrium in the laboratory, or when the amount of one component is too small to measure: K can be calculated from thermodynamic data instead.

6.3 Temperature, $\Delta G^\ominus$ and K

Since $\Delta G^\ominus = \Delta H^\ominus - T\Delta S^\ominus$ and $\Delta G^\ominus = -RT \ln K$, changing the temperature changes both $\Delta G^\ominus$ and K, which is why K is temperature dependent.

Worked example 15 — the Haber process at two temperatures ★

Q. For $N_2(g) + 3H_2(g) \rightleftharpoons 2NH_3(g)$, $\Delta H^\ominus = -92.2$ kJ mol^{-1} and $\Delta S^\ominus = -198.7$ J K^{-1} mol^{-1}. Calculate $\Delta G^\ominus$ and K at 298 K and at 700 K, assuming $\Delta H^\ominus$ and $\Delta S^\ominus$ do not change with temperature, and comment.

298 K: $\Delta G^\ominus = -92\,200 - 298(-198.7) = -33\,000$ J mol^{-1} = **−33.0 kJ mol^{-1}**; $K = e^{33000/(8.31 \times 298)} =$ **6.1×10^5**

700 K: $\Delta G^\ominus = -92\,200 - 700(-198.7) = +46\,900$ J mol^{-1} = **+46.9 kJ mol^{-1}**; $K = e^{-46900/(8.31 \times 700)} =$ **3.2×10^{-4}**

The forward reaction is exothermic, so K falls as the temperature rises, as Le Chatelier predicts. The industrial compromise of about 700 K gives a small K; high pressure and recycling make up for it.

6.4 K and the rate constants

For a reaction that occurs in a single elementary step, A + B ⇌ C + D, the forward rate is k[A][B] and the backward rate is k'[C][D]. At equilibrium these are equal, so k[A][B] = k'[C][D], and

$$K = [C][D] / [A][B] = k / k'$$

This ties together Booklets 4 and 5. A large K means $k \gg k'$. Changing a concentration does not change either rate constant, so K is unchanged. A catalyst increases k and k' by the same factor, so K is unchanged. Temperature increases the rate constant of the step with the larger activation energy more (Arrhenius), so K changes: for an endothermic forward reaction, E_a(forward) > E_a(backward), so k rises faster than k' and K increases.

Worked example 16 — K from rate constants

Q. For a single-step reaction, $k = 2.4 \times 10^{-3}$ and $k' = 6.0 \times 10^{-5}$ (same units) at 300 K. At 320 K, k is 5 times larger and k' is 2 times larger. Calculate K at each temperature and deduce the sign of ΔH for the forward reaction.

300 K: $K = 2.4 \times 10^{-3} / 6.0 \times 10^{-5} =$ **40**; 320 K: $K = (5 \times 2.4 \times 10^{-3}) / (2 \times 6.0 \times 10^{-5}) =$ **100**

K increases with temperature, so **the forward reaction is endothermic**; it has the larger activation energy, which is why k rises more

Model answer: "Explain, in terms of Gibbs energy, why a reaction mixture reaches a position of equilibrium rather than going to completion." (3 marks)

The total Gibbs energy of the mixture decreases as reaction occurs, whether starting from reactants or from products [1]. It therefore passes through a minimum at an intermediate composition [1]. At this minimum $\Delta G = 0$, there is no driving force in either direction and no further net change occurs: this composition is the equilibrium mixture [1].

Examiner traps with $\Delta G^\ominus = -RT \ln K$

- Mixing kJ and J. Convert $\Delta G^\ominus$ to J mol^{-1} (or use $R = 0.00831$ kJ K^{-1} mol^{-1}).
- Using °C instead of K for T.
- Losing the minus sign: a negative $\Delta G^\ominus$ gives a **positive** ln K and $K > 1$.
- Using $\log_{10}$ instead of the natural logarithm, ln.
- Thinking a large K (very negative $\Delta G^\ominus$) means a fast reaction. Rusting has $K \approx 10^{261}$ but is slow.
- Confusing $\Delta G^\ominus$ (pure reactants → pure products, fixed at a given T) with ΔG for a mixture (zero at equilibrium).

7 Key points to memorise

Everything below is either wording that examiners look for or knowledge you must carry into the exam yourself.

A Definitions

- **Reaction quotient, *Q*:** the value of the equilibrium expression using concentrations at any moment (not necessarily at equilibrium).
- **Small-*K* approximation:** when K is very small, $[\text{reactant}]_{\text{equilibrium}} \approx [\text{reactant}]_{\text{initial}}$.
- **Equilibrium (thermodynamic view):** the composition at which the total Gibbs energy is a minimum, $\Delta G = 0$, and total entropy is a maximum.

B Equations and rules

- $Q = K$: at equilibrium; $Q < K$: net reaction right; $Q > K$: net reaction left.
- ICE table: changes in the mole ratio; equilibrium = initial + change; substitute equilibrium concentrations only.
- Solve for x by taking a square root, or by the small-K approximation; no quadratics.
- $\Delta G^{\ominus} = -RT \ln K$ ($\Delta G^{\ominus}$ in J mol^{-1}, T in K); $K = e^{-\Delta G^{\ominus}/RT}$. Negative $\Delta G^{\ominus} \Leftrightarrow K > 1$.
- For a single-step reaction, $K = k/k'$.

C Explanations you will be asked for

- A change in concentration or pressure changes Q, not K; the system reacts until $Q = K$. A change in temperature changes K.
- The approximation is justified because K is very small, so the equilibrium lies far to the left; check that x is under about 5 % of the initial value.
- K can be found from $\Delta G^{\ominus}$ when a reaction is too slow to reach equilibrium or a component is too dilute to measure.
- A catalyst increases k and k' equally, so K is unchanged.

8 Check yourself

Use $R = 8.31$ J K^{-1} mol^{-1} and $T/\text{K} = t/°\text{C} + 273$. Marks are shown in brackets; allow about 1.2 minutes per mark. Full answers are in section 9.

Part A — Multiple choice HL

1. For a reaction mixture, $Q = 25$ and $K = 4.0$. Which is correct?

A The mixture is at equilibrium.

B Net reaction occurs to the right.

C Net reaction occurs to the left.

D K will increase to 25.

2. For $CO(g) + H_2O(g) \rightleftharpoons CO_2(g) + H_2(g)$, $K = 1.00$ at 298 K. A mixture has $[CO] = [H_2O] = 2.00$ and $[CO_2] = [H_2] = 4.00$ mol dm^{-3}. What are Q and the direction of net reaction?

A 0.25; to the right
B 2.0; to the left
C 4.0; to the left
D 4.0; to the right

3. Which statement about Q and K is correct?

A Q has a fixed value at a given temperature.
B Q changes during a reaction until it equals K.
C K changes during a reaction until it equals Q.
D Q can only be calculated at equilibrium.

4. An equilibrium mixture for $N_2O_4(g) \rightleftharpoons 2NO_2(g)$ is compressed to half its volume at constant temperature. Immediately afterwards, which is true?

A $Q = K$
B $Q = 2K$
C $Q = \frac{1}{2}K$
D K doubles

5. 0.50 mol each of $I_2(g)$ and $Br_2(g)$ are placed in a closed flask. At equilibrium the mixture contains 0.80 mol of IBr: $I_2(g) + Br_2(g) \rightleftharpoons 2IBr(g)$. What is K?

A 0.64
B 1.3
C 16
D 64

6. In an ICE table for $N_2 + 3H_2 \rightleftharpoons 2NH_3$, $[NH_3]$ increases by 0.040 mol dm^{-3}. What is the change in $[H_2]$?

A −0.020
B −0.040
C −0.060
D −0.120

7. Which values are substituted into the expression to calculate K?

A initial concentrations
B changes in concentration
C equilibrium concentrations
D equilibrium amounts in moles

8. When is the approximation $[\text{reactant}]_{eqm} \approx [\text{reactant}]_{initial}$ justified?

A when K is very large
B when K is very small
C when $K = 1$
D whenever the temperature is high

9. What are the entropy and Gibbs energy of a system at equilibrium?

A S maximum; G maximum
B S minimum; G maximum
C S maximum; G minimum
D S minimum; G minimum

10. A reaction has $\Delta G^{\ominus} = 0$ at 298 K. What is K?

A 0
B 1
C 2.72
D 298

11. Which combination is correct for a reaction with $K = 3 \times 10^{-9}$?

A $\Delta G^{\ominus}$ negative; mainly products
B $\Delta G^{\ominus}$ negative; mainly reactants
C $\Delta G^{\ominus}$ positive; mainly reactants
D $\Delta G^{\ominus}$ positive; mainly products

12. Which expression gives K from $\Delta G^{\ominus}$?

A $K = e^{\Delta G^{\ominus}/RT}$
B $K = e^{-\Delta G^{\ominus}/RT}$
C $K = -RT \ln \Delta G^{\ominus}$
D $K = 10^{-\Delta G^{\ominus}/RT}$

13. A student calculates K from $\Delta G^{\ominus} = -11.4$ kJ mol^{-1} at 298 K but substitutes −11.4 directly. Which error results?

A K comes out as about 1, instead of about 100.

B K comes out negative.

C K comes out as about 100, instead of about 1.

D No error: the units cancel.

14. For a single-step reaction, the forward rate constant is 3.0×10^{-2} and the backward rate constant is 1.5×10^{-4}. What is K?

A 5.0×10^{-3} **B** 4.5×10^{-6} **C** 2.0×10^{2} **D** 3.0×10^{-2}

15. Why does adding a catalyst not change K?

A It increases k and k' by the same factor.

B It increases only k.

C It changes $\Delta G^{\ominus}$.

D It changes the equilibrium concentrations.

16. The rusting of iron has $K \approx 10^{261}$ at 298 K, yet iron rusts slowly. Which explains this?

A $\Delta G^{\ominus}$ is positive.

B K gives no information about the rate of reaction.

C The reaction is endothermic.

D Rusting does not reach equilibrium.

Part B — Structured questions HL

17. For $H_2O(g) + Cl_2O(g) \rightleftharpoons 2HOCl(g)$, $K = 0.0900$ at 298 K.

(a) Determine whether each mixture (mol dm^{-3}) is at equilibrium: (i) $[H_2O] = 0.100$, $[Cl_2O] = 0.100$, $[HOCl] = 1.00$; (ii) $[H_2O] = 0.49$, $[Cl_2O] = 0.040$, $[HOCl] = 0.042$. [3]

(b) For any mixture not at equilibrium, state the direction of net reaction. [1]

18. For $2SO_2(g) + O_2(g) \rightleftharpoons 2SO_3(g)$, $K = 280$ at a certain temperature. A mixture contains $[SO_2] = 0.100$, $[O_2] = 0.0500$ and $[SO_3] = 0.0500$ mol dm^{-3}. Calculate Q, deduce the direction of net reaction, and state what happens to $[SO_3]$. [3]

19. An equilibrium mixture for $N_2O_4(g) \rightleftharpoons 2NO_2(g)$ at a certain temperature has $[N_2O_4] = 0.050$ and $[NO_2] = 0.020$ mol dm^{-3}. (a) Calculate K. (b) More N_2O_4 is added so that $[N_2O_4]$ momentarily becomes 0.100 mol dm^{-3}. Calculate Q and use it to explain the direction of the shift. [3]

20. 0.400 mol each of CO and H_2O were placed in a 1.00 dm^3 flask: $CO(g) + H_2O(g) \rightleftharpoons CO_2(g) + H_2(g)$. At equilibrium, $[CO_2] = 0.267$ mol dm^{-3}.

(a) Use an ICE table to calculate K. [3]

(b) The experiment is repeated at the same temperature with 0.800 mol of each reactant. State, with a reason, the effect on K and on $[CO_2]$ at equilibrium. [2]

21. 0.80 mol NO and 0.60 mol O_2 reacted in a 2.00 dm^3 container: $2NO(g) + O_2(g) \rightleftharpoons 2NO_2(g)$. At equilibrium the container held 0.40 mol NO_2. Calculate K. [4]

22. ★ 2.00 mol N_2 and 6.00 mol H_2 were placed in a 2.00 dm^3 vessel at 400 °C. At equilibrium, $[NH_3] = 0.050$ mol dm^{-3}. Calculate K for $N_2(g) + 3H_2(g) \rightleftharpoons 2NH_3(g)$. [5]

23. 0.300 mol H_2 and 0.200 mol I_2 were heated in a 2.00 dm^3 flask. At equilibrium the flask contained 0.320 mol HI: $H_2(g) + I_2(g) \rightleftharpoons 2HI(g)$. Calculate K. [4]

24. 0.0100 mol each of SO_2 and Cl_2 were introduced into a 1.00 dm^3 container: $SO_2(g) + Cl_2(g) \rightleftharpoons SO_2Cl_2(g)$, $\Delta H = -84.5$ kJ mol^{-1}. At equilibrium, 0.00800 mol SO_2Cl_2 had formed.

(a) Calculate K. [3]

(b) Predict, with a reason, the effect on $[SO_2Cl_2]$ and on K of lowering the temperature. [2]

(c) Predict, with a reason, the effect on the amount of SO_2Cl_2 and on K of increasing the volume to 1.50 dm^3. [2]

25. For $CO(g) + 2H_2(g) \rightleftharpoons CH_3OH(g)$, $K = 0.500$ at 350 K. At equilibrium, $[CO] = 0.200$ and $[H_2] = 0.155$ mol dm^{-3}. Calculate $[CH_3OH]$. [2]

26. 0.0400 mol dm^{-3} each of H_2 and I_2 are allowed to reach equilibrium at a temperature where $K = 64.0$ for $H_2(g) + I_2(g) \rightleftharpoons 2HI(g)$. Calculate the equilibrium concentrations of all three species. [4]

27. 0.100 mol dm^{-3} each of CO and H_2O react: $CO(g) + H_2O(g) \rightleftharpoons CO_2(g) + H_2(g)$, $K = 4.00$. Calculate the equilibrium concentrations. [4]

28. ★ At a high temperature, $2CO_2(g) \rightleftharpoons 2CO(g) + O_2(g)$ has $K = 1.0 \times 10^{-12}$. The initial $[CO_2]$ is 0.200 mol dm^{-3}.

(a) Calculate $[O_2]$ and $[CO]$ at equilibrium, stating the approximation you make. [4]

(b) Show that the approximation was justified. [1]

29. A weak acid HA has $K = 6.3 \times 10^{-5}$ for $HA(aq) \rightleftharpoons H^+(aq) + A^-(aq)$. Calculate $[H^+]$ in a 0.0500 mol dm^{-3} solution and the percentage of HA that dissociates. State the approximation used. [4]

30. The ionization of water, $H_2O(l) \rightleftharpoons H^+(aq) + OH^-(aq)$, has $K = 1.00 \times 10^{-14}$ at 298 K and 2.92×10^{-14} at 313 K.

(a) Calculate $\Delta G^\ominus$ at 298 K. [2]

(b) Deduce whether the reaction is exothermic or endothermic. [2]

31. (a) Calculate $\Delta G^\ominus$ for a reaction with $K = 1$. (b) For $2NO(g) + O_2(g) \rightleftharpoons 2NO_2(g)$ at 298 K, $K = 1.7 \times 10^{12}$. Calculate $\Delta G^\ominus$ in kJ mol^{-1} and comment on the position of equilibrium. [4]

32. The reaction $2H_2(g) + O_2(g) \rightleftharpoons 2H_2O(l)$ has $\Delta G^\ominus = -474$ kJ mol^{-1} at 298 K. Calculate ln K, and explain why a mixture of hydrogen and oxygen can be kept for years without reacting. [3]

33. A reaction has $\Delta G^\ominus = -5.71$ kJ mol^{-1} at 298 K. Calculate K. Sketch a graph of the total Gibbs energy of the reaction mixture against composition, from pure reactants to pure products, marking the equilibrium position. [4]

34. ★ For a reaction, $\Delta H^\ominus = +58.0$ kJ mol^{-1} and $\Delta S^\ominus = +177$ J K^{-1} mol^{-1}.

(a) Calculate $\Delta G^\ominus$ and K at 298 K. [3]

(b) Calculate $\Delta G^\ominus$ and K at 400 K, and comment on the effect of temperature. [3]

35. A single-step reaction $A + B \rightleftharpoons C + D$ has forward rate constant k and backward rate constant k'.

(a) Show that $K = k/k'$. [2]

(b) Explain, in terms of k and k', why adding a catalyst does not change K. [1]

(c) The forward reaction is exothermic. Explain why K decreases when the temperature rises. [2]

36. ★ Explain, using Q and K, why (a) adding a product to an equilibrium mixture shifts the equilibrium to the left, and (b) raising the temperature of an exothermic equilibrium shifts it to the left. [4]

Part A: 16 marks · Part B: 84 marks · Total: 100 marks (about 2 hours)

9 Answers

Part A

1. C. $Q > K$.

2. C. $Q = (4.00 \times 4.00)/(2.00 \times 2.00) = 4.0 > K$.

3. B.

4. B. Each concentration doubles: $Q = (2[NO_2])^2/(2[N_2O_4]) = 2K$.

5. D. At equilibrium 0.10 mol each of I_2 and Br_2 remain; $0.80^2/(0.10 \times 0.10) = 64$ (the volume cancels).

6. C. $3/2 \times 0.040$.

7. C.

8. B.

9. C.

10. B. $\ln K = 0$.

11. C.

12. B.

13. A. $e^{11\,400/2476} \approx 100$.

14. C.

15. A.

16. B.

Part B

17. (a) (i) $Q = 1.00^2/(0.100 \times 0.100) = 100$ [1]; not at equilibrium [1]. (ii) $Q = 0.042^2/(0.49 \times 0.040) = 0.090 = K$: at equilibrium [1]. (b) (i) $Q > K$, so net reaction to the left [1].

18. $Q = 0.0500^2/(0.100^2 \times 0.0500) = 5.0$ [1]; $Q < K$, so net reaction to the right [1]; $[SO_3]$ increases until $Q = 280$ [1].

19. (a) $K = 0.020^2/0.050 = 8.0 \times 10^{-3}$ [1]. (b) $Q = 0.020^2/0.100 = 4.0 \times 10^{-3}$ [1]; $Q < K$, so net reaction to the right: N_2O_4 decomposes to form more NO_2 until $Q = K$ [1].

20. (a) ICE: CO and H_2O 0.400 → 0.400 − 0.267 = 0.133; CO_2 and H_2 0 → 0.267 [1]; $K = 0.267^2/0.133^2$ [1] = 4.0 [1]. (b) K is unchanged because the temperature is unchanged [1]; $[CO_2]$ doubles to 0.534 mol dm^{-3}, since every concentration doubles and the ratio stays equal to K [1].

21. Initial: [NO] = 0.40, $[O_2] = 0.30$ mol dm^{-3} [1]; $[NO_2] = 0.20$, so changes −0.20, −0.10, +0.20 [1]; equilibrium: [NO] = 0.20, $[O_2] = 0.20$, $[NO_2] = 0.20$ [1]; $K = 0.20^2/(0.20^2 \times 0.20) = 5.0$ [1].

22. Initial: $[N_2] = 1.00$, $[H_2] = 3.00$ mol dm^{-3} [1]; $[NH_3] = +0.050$, so N_2 −0.025 and H_2 −0.075 [1]; equilibrium: $[N_2] = 0.975$, $[H_2] = 2.925$ [1]; $K = [NH_3]^2/[N_2][H_2]^3$ [1] $= 0.050^2/(0.975 \times 2.925^3) = 1.0 \times 10^{-4}$ [1].

23. Initial: $[H_2] = 0.150$, $[I_2] = 0.100$ mol dm^{-3} [1]; [HI] = 0.160, so each reactant fell by 0.080 [1]; $[H_2] = 0.070$, $[I_2] = 0.020$ [1]; $K = 0.160^2/(0.070 \times 0.020) = 18$ [1].

24. (a) Equilibrium: $[SO_2] = [Cl_2] = 0.0100 - 0.00800 = 0.00200$; $[SO_2Cl_2] = 0.00800$ [1]; $K = [SO_2Cl_2]/[SO_2][Cl_2]$ [1] $= 0.00800/(0.00200)^2 = 2.0 \times 10^3$ [1]. (b) Forward reaction exothermic, so lowering T shifts right: $[SO_2Cl_2]$ increases and K increases [2]. (c) Larger volume favours the side with more gas molecules (2 vs 1): the amount of SO_2Cl_2 decreases [1]; K unchanged at constant temperature [1].

25. $[CH_3OH] = K[CO][H_2]^2 = 0.500 \times 0.200 \times 0.155^2$ [1] $= 2.40 \times 10^{-3}$ mol dm^{-3} [1].

26. ICE with change $-x$, $-x$, $+2x$ [1]; √64.0: $2x/(0.0400 - x) = 8.00$ [1]; $x = 0.0320$ [1]; [HI] = 0.0640, $[H_2] = [I_2] = 0.0080$ mol dm^{-3} [1].

27. ICE with change $-x$, $-x$, $+x$, $+x$ [1]; √4.00: $x/(0.100 - x) = 2.00$ [1]; $x = 0.0667$ [1]; $[CO_2] = [H_2] = 0.0667$, $[CO] = [H_2O] = 0.0333$ mol dm^{-3} [1].

28. (a) Let $[O_2] = x$, $[CO] = 2x$, $[CO_2] = 0.200 - 2x \approx 0.200$ because K is very small [1]; $(2x)^2x/0.200^2 = 1.0 \times 10^{-12}$ [1]; $4x^3 = 4.0 \times 10^{-14}$, $x = 2.2 \times 10^{-5}$ [1]; $[O_2] = 2.2 \times 10^{-5}$ and $[CO] = 4.3 \times 10^{-5}$ mol dm^{-3} [1]. (b) $2x = 4.3 \times 10^{-5}$ is only 0.02 % of 0.200 [1].

29. $[HA] \approx 0.0500$ because K is small [1]; $x^2 = 6.3 \times 10^{-5} \times 0.0500 = 3.15 \times 10^{-6}$ [1]; $[H^+] = 1.8 \times 10^{-3}$ mol dm^{-3} [1]; dissociation = $1.8 \times 10^{-3}/0.0500 \times 100 = 3.5$ % [1].

30. (a) $\Delta G^\ominus = -8.31 \times 298 \times \ln(1.00 \times 10^{-14})$ [1] $= +7.98 \times 10^4$ J $mol^{-1} = +79.8$ kJ mol^{-1} [1]. (b) K increases with temperature [1], so the forward reaction is endothermic [1].

31. (a) $\Delta G^\ominus = -RT \ln 1 = 0$ [1]. (b) $\Delta G^\ominus = -8.31 \times 298 \times \ln(1.7 \times 10^{12})$ [1] $= -69.7$ kJ mol^{-1} [1]; large and negative ($K \gg 1$), so the equilibrium lies far to the right [1].

32. $\ln K = 474\,000/(8.31 \times 298)$ [1] = 191 [1]; K is enormous, but the activation energy is high, so the rate at room temperature is negligible: K gives no information about rate [1].

33. ln $K = 5710/(8.31 \times 298) = 2.31$ [1]; $K = 10.0$ [1]; sketch: curve falling from pure reactants and rising towards pure products [1], with its minimum (equilibrium) closer to the products [1].

34. (a) $\Delta G^{\ominus} = 58\,000 - 298 \times 177 = +5254$ J mol^{-1} = +5.25 kJ mol^{-1} [1]; $K = e^{-5254/(8.31 \times 298)}$ [1] = 0.12 [1]. (b) $\Delta G^{\ominus} = 58\,000 - 400 \times 177 = -12\,800$ J mol^{-1} = −12.8 kJ mol^{-1} [1]; $K = e^{12\,800/(8.31 \times 400)} = 47$ [1]; for this endothermic reaction with positive ΔS, a higher temperature makes $\Delta G^{\ominus}$ negative and K larger, shifting the equilibrium to the products [1].

35. (a) At equilibrium forward rate = backward rate: $k[A][B] = k'[C][D]$ [1]; rearranging, $[C][D]/[A][B] = K = k/k'$ [1]. (b) The catalyst increases k and k' by the same factor, so their ratio is unchanged [1]. (c) For an exothermic reaction, E_a(backward) > E_a(forward) [1]; a temperature rise increases k' by a larger factor than k, so $k/k' = K$ decreases [1].

36. (a) Adding product increases the numerator, so Q becomes greater than K [1]; net reaction to the left until Q falls back to K [1]. (b) A temperature rise does not change Q but decreases K for an exothermic reaction [1]; now Q > the new K, so net reaction is to the left until Q equals the new K [1].

Where this fits in Reactivity 2

- **Booklets 1–2** — Reactivity 2.1: how much? **Booklets 3–4** — Reactivity 2.2: how fast? **Booklet 5** — Reactivity 2.3.1–2.3.4 (SL + HL): how far? **Booklet 6 (this booklet)** — Reactivity 2.3.5–2.3.7 (HL): Q, equilibrium calculations and Gibbs energy. This completes Reactivity 2.
- **Next:** Reactivity 3.1 uses the equilibrium law and the small-K approximation to calculate the pH of weak acids, weak bases and buffers.

These notes are a free resource, shared for any IB student who finds them useful.

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