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GIBBS FREE ENERGY

Two factors determine whether a reaction is feasible:

- **Enthalpy change (ΔH)** (exothermic favourable)
- **Entropy change** (which is temperature dependent) **($T\Delta S$)** (entropy increase favourable)

Combined in this equation where ΔH is Gibbs free energy change

$$\Delta G = \Delta H - T\Delta S$$

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$\Delta G \leq 0$ reaction is **feasible**

$\Delta G > 0$ reaction is **NOT feasible**

Feasible means reaction CAN take place although it might not (e.g. activation energy too high)

The term 'spontaneous' sometime used for feasible

ΔH	ΔS	How ΔG varies with temperature	How feasibility varies with temperature
–ve	+ve	ΔG always –ve	feasible at all temperatures
–ve	–ve	lower T: ΔG –ve higher T: ΔG +ve	lower T: feasible higher T: not feasible
+ve	+ve	lower T: ΔG +ve higher T: ΔG –ve	lower T: not feasible higher T: feasible
+ve	–ve	ΔG always +ve	never feasible at any temperature

EXAMPLE 1

Zinc carbonate decomposes on heating: $ZnCO_3(s) \rightarrow ZnO(s) + CO_2(g)$

	$ZnCO_3(s)$	$ZnO(s)$	$CO_2(g)$
Δ_fH (kJ mol^{-1})	-812	-348	-394
S (J mol^{-1} K^{-1})	83.0	44.0	214

a) Calculate ΔH, ΔS and ΔG for this reaction at 298 K.

b) Is the reaction feasible at 298 K?

c) Give the temperature range in which the decomposition of $ZnCO_3$ is feasible.

a) ΔH = [Sum of Δ_fH products] – [Sum Δ_fH reactants]

= [–348 – 394] – [–812]

= +70 kJ mol^{-1}

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ΔS = [Sum of S products] – [Sum S reactants]

= [44 + 214] – [–83]

= +175 J mol^{-1} K^{-1}

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$\Delta G = \Delta H - T\Delta S$

$= 70 - 298\left(\frac{175}{1000}\right)$

$= +17.9$ kJ mol^{-1}

reaction is NOT feasible at 298K

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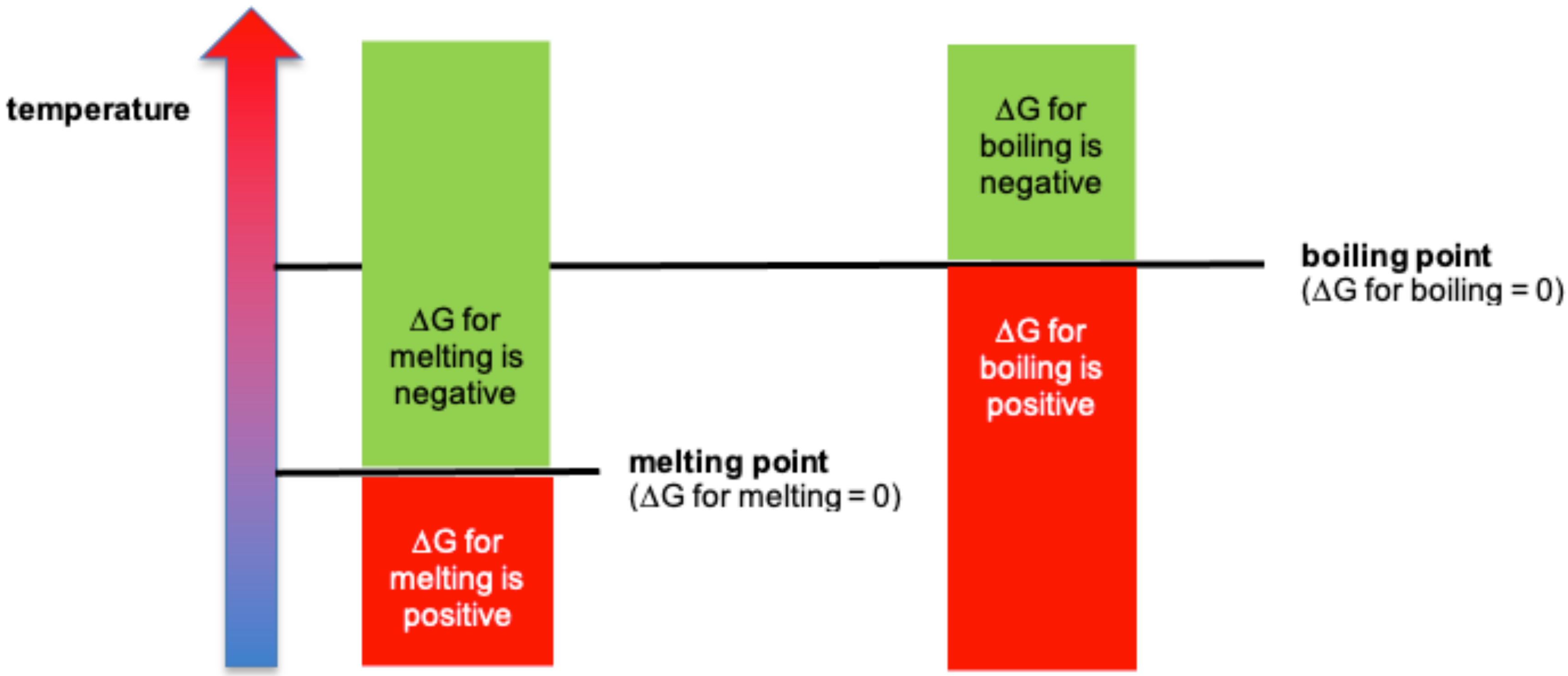
when $\Delta G = 0$

$0 = \Delta H - T\Delta S$ $\quad \Delta H = T\Delta S$ $\quad T = \frac{\Delta H}{\Delta S}$

$T = \frac{\Delta H}{\Delta S} = \frac{70}{\frac{175}{1000}}$ $= 400$ K (2 sf)

reaction is feasible when $T \geq 400$ K

Changes of state are controlled in the same way.



EXAMPLE 2

The enthalpy change for melting potassium chloride is +25.5 kJ mol^{-1}, and the entropy change is +24.5 J mol^{-1} K^{-1}. Calculate the temperature at which potassium chloride melts.

when $\Delta G = 0$

$$0 = \Delta H - T\Delta S \qquad \Delta H = T\Delta S \qquad T = \frac{\Delta H}{\Delta S}$$

$$T = \frac{\Delta H}{\Delta S} = \frac{25.5}{\frac{24.5}{1000}} = 1040\ K$$

EXAMPLE 3

The enthalpy of vaporisation of ethanol is +43.5 kJ mol^{-1}. The boiling point of ethanol is 78°C. Calculate the entropy change for the vaporisation of ethanol.

when $\Delta G = 0$

$$0 = \Delta H - T\Delta S \qquad \Delta H = T\Delta S \qquad \Delta S = \frac{\Delta H}{T}$$

$$\Delta S = \frac{\Delta H}{T} = \frac{43.5}{351} = 0.124 \text{ kJ mol}^{-1}\text{ K}^{-1} = 124 \text{ J mol}^{-1}\text{ K}^{-1}$$