Chemistry

For the IB Diploma

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Chapter 15

Entropy and spontaneity

Entropy

Entropy (*S*) a measure of the disorder of a system (how the matter is dispersed / distributed) or how the available energy is distributed among the particles. Standard entropy ($S^{\ominus}$) is the entropy of a substance at 100 kPa and 298.15 K; units are J K^{-1} mol^{-1}. $\Delta S^{\ominus}$ is the entropy change under standard conditions – a positive value indicates an increase in entropy, i.e., the system is more disordered/the energy is more spread out (less concentrated).

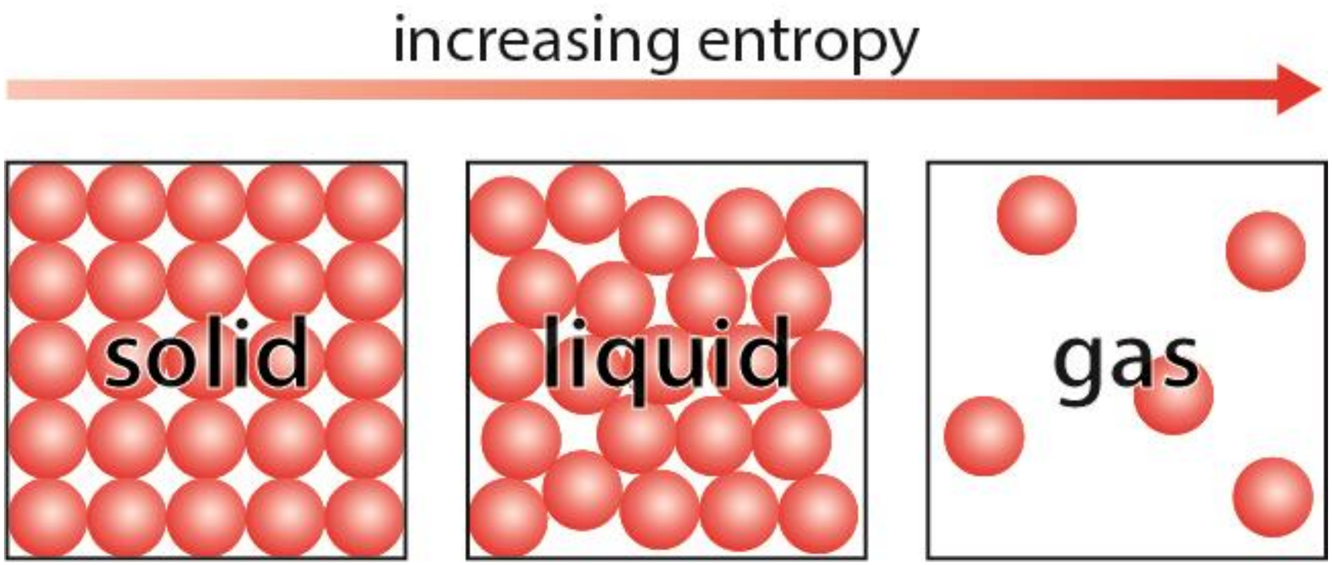

Figure 15.1: In a solid, the particles vibrate about mean positions; in a liquid, the particles move around each other; in a gas, the particles move at high speeds in all directions.

Working out entropy of reactions

Reaction	Entropy	ΔS	Explanation
$N_2(g) + 3H_2(g) \longrightarrow 2NH_3(g)$	Decrease	–	Four moles of gas on the left-hand side are converted into two moles of gas on the right-hand side; a decrease in the number of moles of gas is a decrease in disorder; therefore, the energy can be distributed in fewer ways in the products.
$CaCO_3(s) \longrightarrow CaO(s) + CO_2(g)$	Increase	+	One mole of solid becomes one mole of solid and one mole of gas; increase in the number of moles of gas = an increase in disorder.
$CH_4(g) + 2O_2(g) \longrightarrow CO_2(g) + 2H_2O(l)$	Decrease	–	Three moles of gas are converted into one mole of gas; decrease in the number of moles of gas = decrease in disorder.
$C_2H_4(g) + H_2(g) \longrightarrow C_2H_6(g)$	Decrease	–	Two moles of gas are converted into one mole of gas; decrease in the number of moles of gas = decrease in disorder.

Entropy calculations and Gibbs energy calculations

Entropy change = total entropy of products − total entropy of reactants

$$\Delta S^\ominus = \sum S^\ominus_{\text{products}} - \sum S^\ominus_{\text{reactants}}$$

ΔG is called the Gibbs energy change, or the free energy change.

Under standard conditions (pressure = 100 kPa), we have $\Delta G^\ominus$, which is the standard Gibbs energy change:

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

Work out the spontaneity of a reaction using ΔH and ΔS

$\Delta H^{\ominus}$	$\Delta S^{\ominus}$	$-T\Delta S^{\ominus}$	$\Delta G^{\ominus}$	**Spontaneous?**
Negative	Positive	Negative	Negative	At all temperatures
Positive	Positive	Negative	Becomes more negative as temperature increases	Becomes more spontaneous as temperature increases
Negative	Negative	Positive	Becomes less negative as temperature increases	Becomes less spontaneous as temperature increases
Positive	Negative	Positive	Positive	Never

Graphs showing Gibbs energy and the relationship with equilibrium

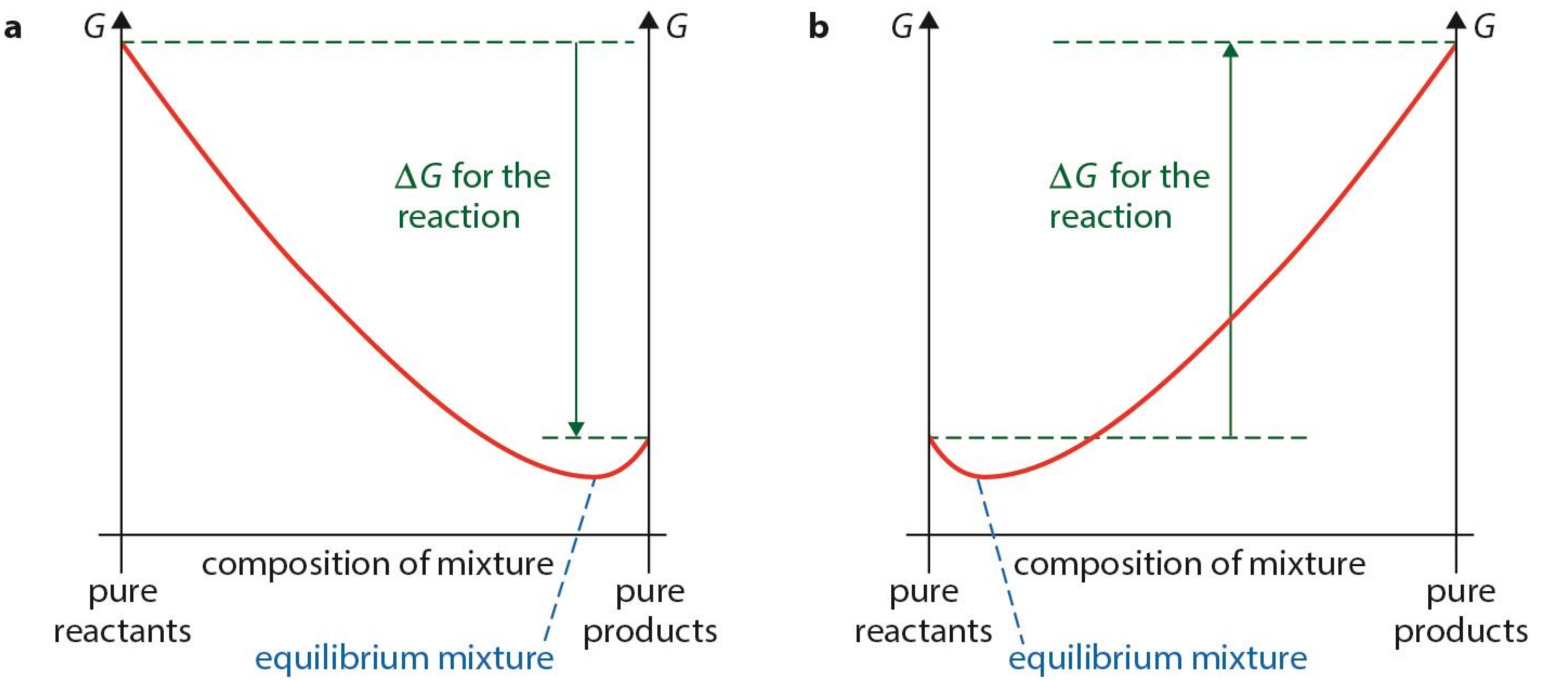

Figure 15.2: **a** $\Delta G^{\ominus}$ is negative and the position of equilibrium lies closer to the products; **b** $\Delta G^{\ominus}$ is positive and the position of equilibrium lies closer to the reactants.