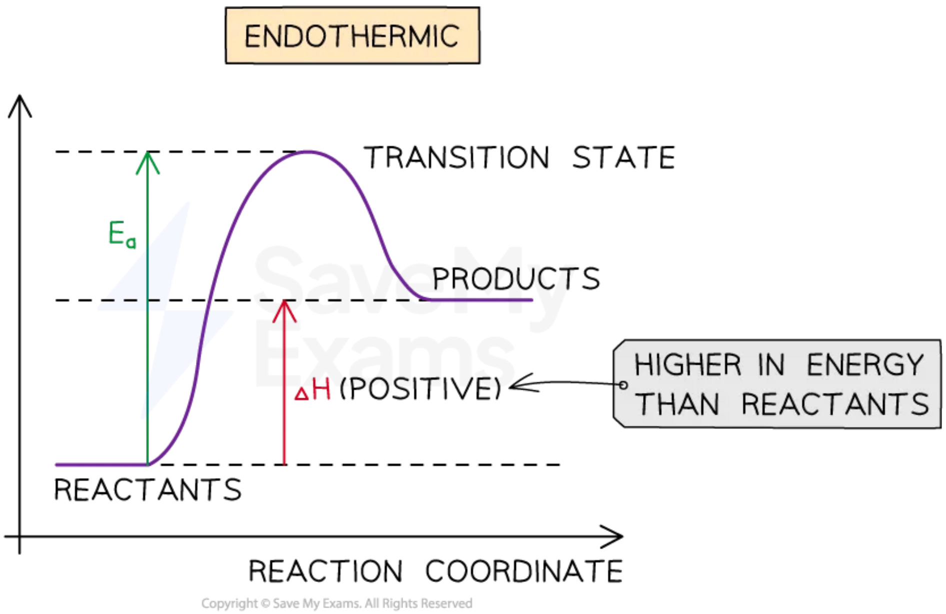
Entropy

- You may have wondered why it is that endothermic reactions occur at all, after all, what can be the driving force behind endothermic reactions if the products end up in a less stable, higher energy state?
- Although the majority of chemical reactions we experience every day are exothermic, $\Delta H^{\ominus}$ alone is not enough to explain why endothermic reactions occur

Endothermic reaction profile



The driving force behind chemical reactions cannot be explained by enthalpy changes alone as it does not sense for chemical to end up in a less stable higher energy state in endothermic reactions

- The answer is entropy

Chaos in the universe

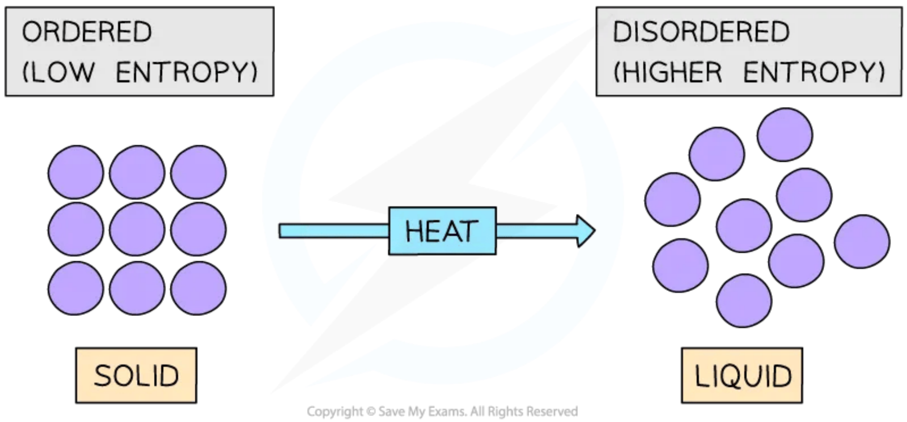
- The entropy (S) of a given system is the number of possible arrangements of the particles and their energy in a given system
  - In other words, it is a measure of how disordered or chaotic a system is
- When a system becomes more disordered, its entropy will increase
- An increase in entropy means that the system becomes energetically more stable
- For example, during the thermal decomposition of calcium carbonate ($CaCO_3$) the entropy of the system increases:

$CaCO_3$ (s) → CaO (s) + CO_2 (g)

- In this decomposition reaction, a gas molecule (CO_2) is formed
- The CO_2 gas molecule is more disordered than the solid reactant ($CaCO_3$), as it is constantly moving around
- As a result, the system has become more disordered and there is an increase in entropy
- Another typical example of a system that becomes more disordered is when a solid melts
  - For example, melting ice to form liquid water:
    H_2O (s) → H_2O (l)

- The water molecules in ice are in fixed positions and can only vibrate about those positions
- In the liquid state, the particles are still quite close together but are arranged more randomly, in that they can move around each other
- Water molecules in the liquid state are therefore more disordered
- Thus, for a given substance, the entropy increases when its solid form melts into a liquid
- In both examples, the system with the higher entropy will be energetically favourable (as the energy of the system is more spread out when it is in a disordered state)

Low entropy to high entropy



Melting a solid will cause the particles to become more disordered resulting in a higher entropy state

Calculating Standard Entropy Changes

- The standard molar enthalpy values, S°, relate to standard conditions of temperature and pressure
- The entropy change, ΔS°, can be calculated from thermodynamic data using the following equation:

ΔS°_{298}(reaction) = ΣS°_{298}(products) - ΣS°_{298}(reactants)

- This equation is provided in the data booklet
- The units of $\Delta S_{system}^{\circ}$ are in J K^{-1} mol^{-1}
- Entropy will change depending on the state of the matter
  - Taking water as an example the values for S° will be different for the liquid and gaseous phases
    - $S^{\circ}_{298}(H_2O\ (l))$ = 70.0 J K^{-1} mol^{-1}
    - $S^{\circ}_{298}(H_2O\ (g))$ = 188.8 J K^{-1} mol^{-1}
- When calculating ΔS°, the coefficients used to balance the equation must be applied when calculating the overall entropy change
- For example, when calculating the ΔS° for the reaction below we need to double the value for S° (NO (g))
  - $N_2O_4\ (g) \rightarrow 2NO_2\ (g)$
  - ΔS°_{298}(reaction) = ΣS°_{298}(products) - ΣS°_{298}(reactants)
  - $\Delta S^{\circ} = [(2 \times S^{\circ}_{298}(NO_2)] - S^{\circ}_{298}(N_2O_4)$

Worked Example

What is the entropy change when calcium carbonate decomposes?

$CaCO_3\ (s) \rightarrow CaO\ (s) + CO_2\ (g)$

- $S^{\ominus}_{298}(CaCO_3\ (s))$ = 92.9 J K−1 mol−1
- $S^{\ominus}_{298}(CaO\ (s))$ = 39.7 J K−1 mol−1
- $S^{\ominus}_{298}(CO_2\ (g))$ = 213.6 J K−1 mol−1

Answer:

Step 1: Write out the equation to calculate $\Delta S^{\ominus}_{298}$(reaction)

- $\Delta S^{\ominus}_{298}$(reaction) = $\Sigma S^{\ominus}_{298}$(products) - $\Sigma S^{\ominus}_{298}$(reactants)

Step 2: Substitute in formulas and then values for $S^{\ominus}$

- $\Delta S_{\ominus 298}$(reaction) = $[S^{\ominus}_{298}(CaO) + S^{\ominus}_{298}(CO_2)] - S^{\ominus}_{298}(CaCO_3)$
- $\Delta S^{\ominus}$(reaction) = (39.7 + 213.6) - 92.9
- $\Delta S^{\ominus}$(reaction) = +160.4 J K^{-1} mol^{-1}

Worked Example

What is the entropy change when ammonia is formed from nitrogen and hydrogen?

$N_2\ (g) + 3H_2\ (g) \rightleftharpoons 2NH_3\ (g)$

- $S^{\ominus}_{298}(N_2\ (g))$ = 191.6 J K^{-1} mol^{-1}
- $S^{\ominus}_{298}(H_2\ (g))$ = 131 J K^{-1} mol^{-1}
- $S^{\ominus}_{298}(NH_3)$ = 192.3 J K^{-1} mol^{-1}

Answer:

Step 1: Write out the equation to calculate $\Delta S^{\ominus}_{298}$(reaction)

- $\Delta S^{\ominus}_{298}$(reaction) = $\Sigma S^{\ominus}_{298}$(products) - $\Sigma S^{\ominus}_{298}$(reactants)

Step 2: Substitute in formulas and then values for $S^{\ominus}$ taking into account the coefficients

- $\Delta S^{\ominus}_{298}$(reaction) = $[2 \times S^{\ominus}_{298}(NH_3)] - [S^{\ominus}_{298}(N_2) + (3 \times S^{\ominus}_{298}(H_2))]$
- $\Delta S^{\ominus}_{298}$(reaction) = [2 x 192.3] - [191.6 + (3 x 131)]
- $\Delta S^{\ominus}_{298}$(reaction) = 384.6 - 584.6
- $\Delta S^{\ominus}_{298}$(reaction) = -200 J K^{-1} mol^{-1}

Gibbs Free Energy

- The feasibility of a reaction is determined by two factors, the enthalpy change and the entropy change
- The two factors come together in a fundamental thermodynamic concept called the Gibbs free energy (G)
- The Gibbs equation is:

$\Delta G^{\ominus} = \Delta H_{reaction}^{\ominus} - T\Delta S_{system}^{\ominus}$

- The units of $\Delta G^{\ominus}$ are in kJ mol^{-1}
- The units of $\Delta H_{reaction}^{\ominus}$ are in kJ mol^{-1}
- The units of T are in K
- The units of $\Delta S_{system}^{\ominus}$ are in J K^{-1} mol^{-1} (and must therefore be converted to kJ K^{-1} mol^{-1} by dividing by 1000)

Calculating $\Delta G^{\ominus}$

- There are two ways you can calculate the value of $\Delta G^{\ominus}$

1. From the Gibbs equation, using enthalpy change, $\Delta H^{\ominus}$, and entropy change, $\Delta S^{\ominus}$, values
2. From $\Delta G^{\ominus}$ values of all the substances present

Worked Example

$\Delta G^{\ominus}$ from $\Delta H^{\ominus}$ and $\Delta S^{\ominus}$ values

Calculate the free energy change for the following reaction at 298 K:
$2NaHCO_3 (s) \rightarrow Na_2CO_3 (s) + H_2O (l) + CO_2 (g)$

- $\Delta H^{\ominus}$ = +135 kJ mol^{-1}
- $\Delta S^{\ominus}$ = +344 J K-1 mol^{-1}

Answer:

- Step 1: Convert the entropy value in kilojoules
    - $\Delta S^{\ominus} = \frac{+344 \text{ J K}^{-1} \text{ mol}^{-1}}{1000}$ = +0.344 kJ K^{-1} mol^{-1}
- Step 2: Substitute the terms into the Gibbs Equation
    - $\Delta G^{\ominus} = \Delta H_{reaction}^{\ominus} - T\Delta S_{system}^{\ominus}$
    - $\Delta G^{\ominus}$ = +135 – (298 x 0.344)
    - $\Delta G^{\ominus}$ = +32.49 kJ mol^{-1}

Worked Example

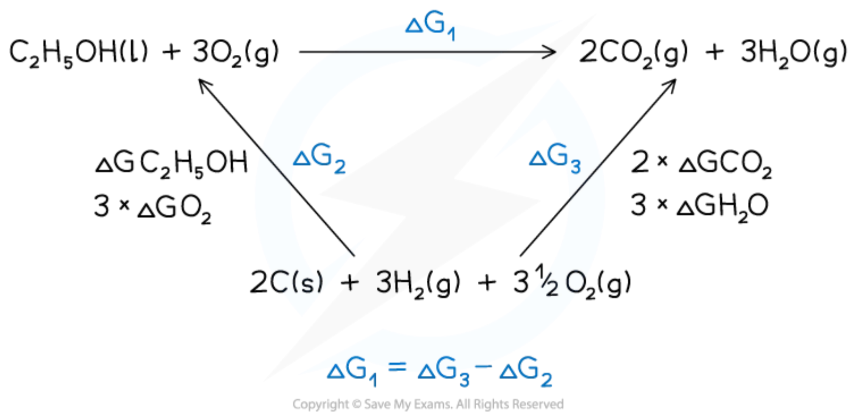
$\Delta G^{\ominus}$ from other $\Delta G^{\ominus}$ values

What is the standard free energy change, $\Delta G^{\ominus}$, for the following reaction?
$C_2H_5OH (l) + 3O_2 (g) \rightarrow 2CO_2 (g) + 3H_2O (g)$

Substance	$\Delta G^{\ominus}$ kJ mol^{-1}
C_2H_5OH (l)	-175
O_2 (g)	0
CO_2 (g)	-394
H_2O (g)	-229

Answer:

- This can be calculated in the same way as you complete enthalpy calculations
    - $\Delta G^{\ominus} = \Sigma\Delta G_{products}^{\ominus} - \Sigma\Delta G_{reactants}^{\ominus}$
    - $\Delta G^{\ominus}$ = [(2 x CO_2) + (3 x H_2O)] – [(C_2H_5OH) + (3 x O_2)]
    - $\Delta G^{\ominus}$ = [(2 x -394) + (3 x -229)] – [-175 + 0]
    - $\Delta G^{\ominus}$ = -1300 kJ mol^{-1}
- This can also be done by drawing a Hess cycle - find the way that is best for you



Examiner Tips and Tricks

- The idea of free energy is what's 'leftover' to do useful work when you've carried out the reaction
- The enthalpy change is the difference between the energy you put in to break the chemical bonds and the energy out when making new bonds
- The entropy change is the 'cost' of carrying out the reaction, so free energy is what you are left with!

Spontaneous Reactions

- Gibbs free energy provides an effective way of focusing on a reaction system at constant temperature and pressure to determine its spontaneity
- For a reaction to be spontaneous, Gibbs free energy must have a negative value ($\Delta G^{\ominus} \leq 0$)
- We can use the Gibbs equation to calculate whether a reaction is spontaneous / feasible or not
  $\Delta G^{\ominus} = \Delta H_{reaction}^{\ominus} - T\Delta S_{system}^{\ominus}$
- When $\Delta G^{\ominus}$ is negative, the reaction is spontaneous / feasible and likely to occur
- When $\Delta G^{\ominus}$ is positive, the reaction is not spontaneous / feasible and unlikely to occur
- Depending on the value for ΔH and ΔS we can determine whether the reaction is spontaneous at a given temperature (T)
- We can also look at the values for enthalpy change, ΔH, and entropy change, ΔS

Worked Example

Determining if a reaction is feasible / spontaneous

1. Calculate the Gibbs free energy change for the following reaction at 298 K
2. Determine whether the reaction is feasible.
   $2Ca\ (s) + O_2\ (g) \rightarrow 2CaO\ (s)$ $\Delta H = -635.5\ kJ\ mol^{-1}$

- $S^{\ominus}[Ca(s)] = 41.00\ J\ K^{-1}\ mol^{-1}$
- $S^{\ominus}[O2(g)] = 205.0\ J\ K^{-1}\ mol^{-1}$
- $S^{\ominus}[CaO(s)] = 40.00\ J\ K^{-1}\ mol^{-1}$

Answer 1:

Step1: Calculate $\Delta S_{system}^{\ominus}$

- $\Delta S_{system}^{\ominus} = \Sigma\Delta S_{products}^{\ominus} - \Sigma\Delta S_{reactants}^{\ominus}$
- $\Delta S_{system}^{\ominus} = (2 \times \Delta S^{\ominus}\ [CaO(s)]) - (2 \times \Delta S^{\ominus}\ [Ca(s)] + \Delta S^{\ominus}\ [O_2(g)])$

- ○ $= (2 \times 40.00) – (2 \times 41.00 + 205.0)$
- ○ $= -207.0 \text{ J K}^{-1} \text{ mol}^{-1}$

Step 2: Convert $\Delta S^{\ominus}$ to $\text{kJ K}^{-1} \text{ mol}^{-1}$

- $\Delta S_{system}^{\ominus} = \dfrac{-207.0 \text{ J K}^{-1} \text{ mol}^{-1}}{1000} = -0.207 \text{ kJ mol}^{-1}$

Step 3: Calculate $\Delta G^{\ominus}$

- $\Delta G^{\ominus} = \Delta H_{reaction}^{\ominus} – T\Delta S_{system}^{\ominus}$

$\Delta G^{\ominus} = -635.5 – (298 \times -0.207)$

$= –573.8 \text{ kJ mol}^{-1}$

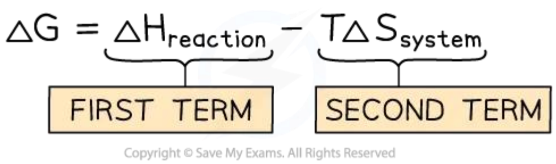
Answer 2:

- Since $\Delta G^{\ominus}$ is negative, the reaction is feasible

Factors affecting ΔG and the spontaneity / feasibility of a reaction

- We can also look at the values for ΔH and ΔS to determine whether the reaction is spontaneous / feasible at a given temperature (T)
- The Gibbs equation will be used to explain what will affect the spontaneity / feasibility of a reaction for exothermic and endothermic reactions

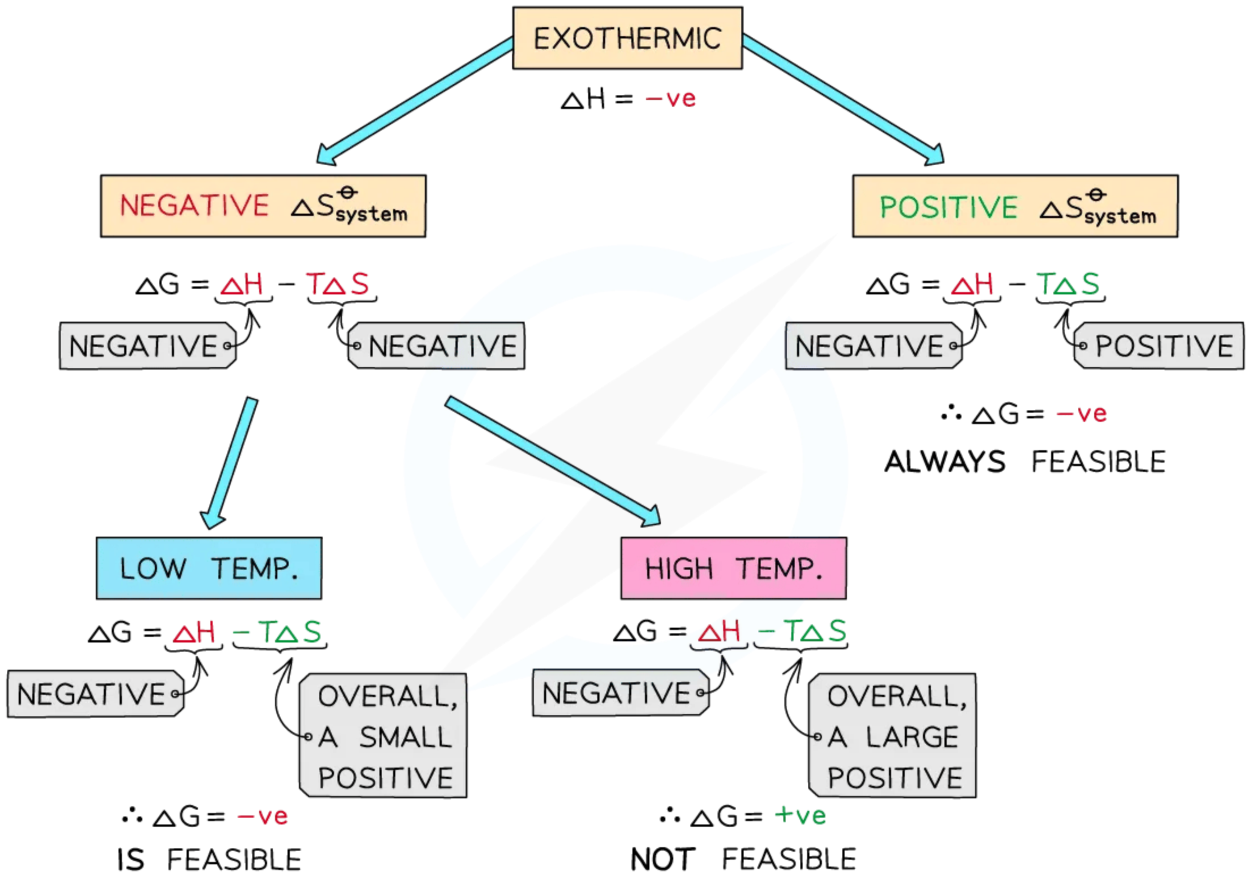
Gibbs free energy equation



Exothermic reactions

- In exothermic reactions, $\Delta H_{reaction}^{\ominus}$ is negative
- If the $\Delta S_{system}^{\ominus}$ is positive:
  - Both the first and second terms will be negative
  - Resulting in a negative $\Delta G^{\ominus}$ so the reaction is feasible
  - Therefore, regardless of the temperature, an exothermic reaction with a positive $\Delta S_{system}^{\ominus}$ will always be feasible
- If the $\Delta S_{system}^{\ominus}$ is negative:
  - The first term is negative and the second term is positive
  - At very high temperatures, the $–T\Delta S_{system}^{\ominus}$ will be very large and positive and will overcome $\Delta H_{reaction}^{\ominus}$
  - Therefore, at high temperatures $\Delta G^{\ominus}$ is positive and the reaction is not feasible
- Since the relative size of an entropy change is much smaller than an enthalpy change, it is unlikely that $T\Delta S > \Delta H$ as temperature increases
- These reactions are therefore usually spontaneous under normal conditions

Flow chart to determine the feasibility of exothermic reactions

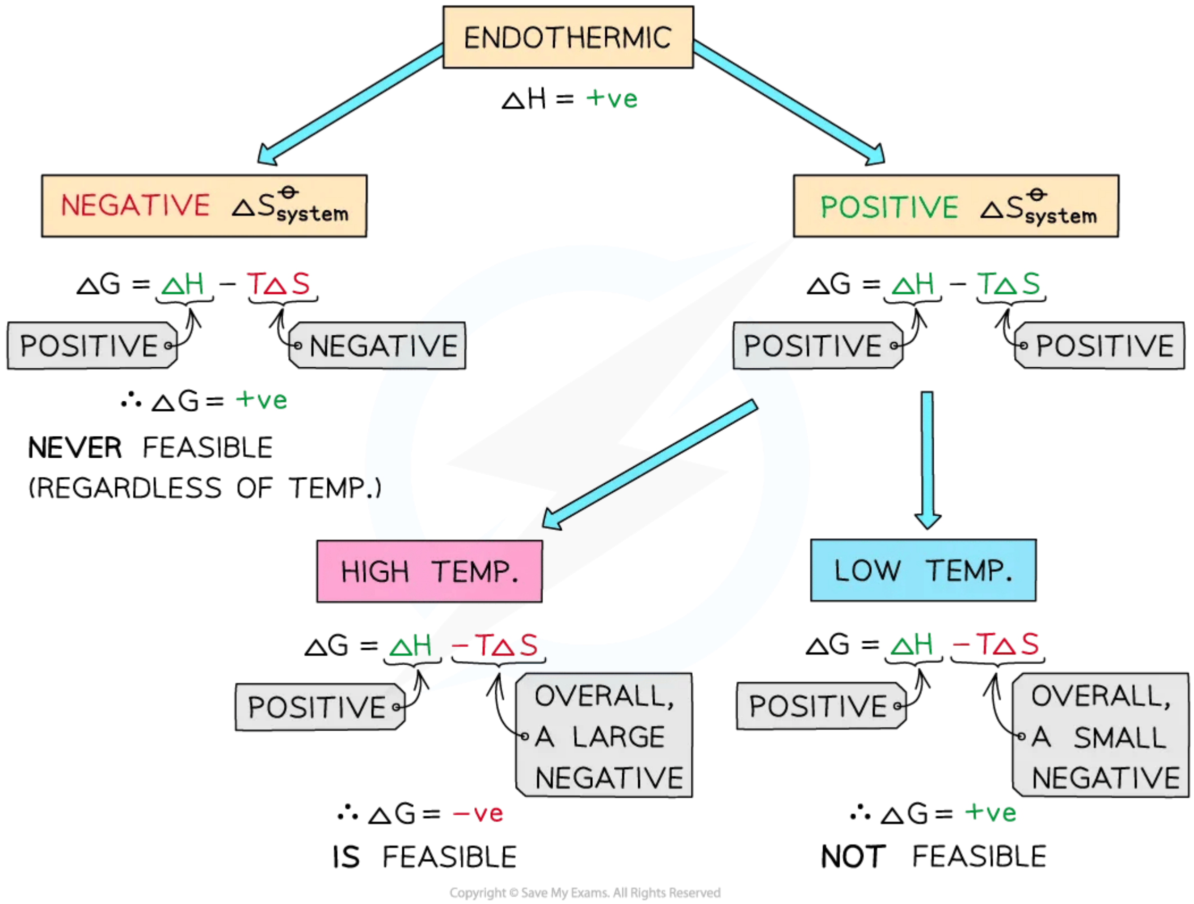


The diagram shows under which conditions exothermic reactions are feasible

Endothermic reactions

- In endothermic reactions, $\Delta H_{reaction}^{\ominus}$ is positive
- If the $\Delta S_{system}^{\ominus}$ is negative:
  - Both the first and second term will be positive
  - Resulting in a positive $\Delta G^{\ominus}$ so the reaction is not feasible
  - Therefore, regardless of the temperature, endothermic with a negative $\Delta S_{system}^{\ominus}$ will never be feasible
- If the $\Delta S_{system}^{\ominus}$ is positive:
  - The first term is positive and the second term is negative
  - At low temperatures, the $-T\Delta S_{system}^{\ominus}$ will be small and negative and will not overcome the larger $\Delta H_{reaction}^{\ominus}$
  - Therefore, at low temperatures $\Delta G^{\ominus}$ is positive and the reaction is not feasible
  - The reaction is more feasible at high temperatures as the second term will become negative enough to overcome the ΔHreaction⊖ resulting in a negative $\Delta G^{\ominus}$
- This tells us that for certain reactions which are not feasible at room temperature, they can become feasible at higher temperatures
  - An example of this is found in metal extractions, such as the extraction if iron in the blast furnace, which will be unsuccessful at low temperatures but can occur at higher temperatures (~1500 °C in the case of iron)

Flow chart to determine the feasibility of endothermic reactions



The diagram shows under which conditions endothermic reactions are feasible

Summary of factors affecting Gibbs free energy

If ΔH	And if ΔS	Then ΔG is	Spontaneous?	Because
is negative < 0 exothermic	is positive > 0 more disorder	always negative < 0	Always	Forward reaction spontaneous at any T
is positive > 0 endothermic	is negative < 0 more order	always positive > 0	Never	Reverse reaction spontaneous at any T
is negative < 0 exothermic	is negative < 0 more order	negative at low T positive high T	Dependent on T	Spontaneous only at low T TΔS < H
is positive > 0 endothermic	is positive > 0 more disorder	negative at high T positive low T	Dependent on T	Spontaneous only at high T TΔS > H

Temperature & Spontaneity

- Rearranging the Gibbs equation allows you to determine the temperature at which a non-spontaneous reaction become feasible
  $\Delta G^{\ominus} = \Delta H_{reaction}^{\ominus} - T\Delta S_{system}^{\ominus}$
- Remember, for a reaction to be feasible $\Delta G^{\ominus}$must be zero or negative
  - $0 = \Delta H^{\ominus} - T\Delta S^{\ominus}$
  - $\Delta H^{\ominus} = T\Delta S^{\ominus}$
  - T = $\frac{\Delta H^{\theta}}{\Delta S^{\theta}}$

Worked Example

At what temperature will the reduction of aluminium oxide with carbon become spontaneous?

Al_2O_3 (s) + 3C (s)→ 2Al (s) + 3CO (g)

$\Delta H^{\ominus}$ = +1336 kJ mol^{-1}

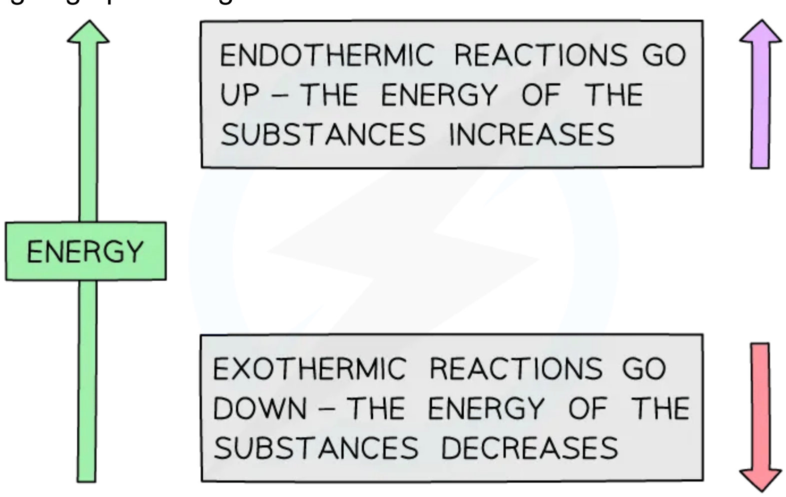
$\Delta S^{\ominus}$ = +581 J K-1 mol^{-1}

Answer:

- If $\Delta G^{\ominus}$ = 0 then T = $\frac{\Delta H^{\theta}}{\Delta S^{\theta}}$
- Convert $\Delta S^{\ominus}$ to kJ K^{-1} mol^{-1} by dividing by 1000
- T = $\frac{1336}{\left(\frac{581}{1000}\right)}$ = 2299 K

Born-Haber Cycles

- A Born-Haber cycle is a specific application of Hess's Law for ionic compounds and enables us to calculate lattice enthalpy, which cannot be found by experiment
- The basic principle of drawing the cycle is to construct a diagram in which energy increases going up the diagram



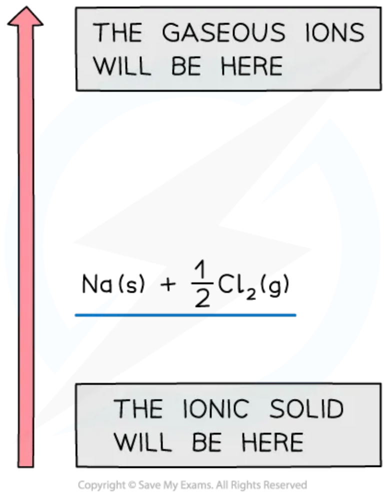
The basic principle of a Born-Haber cycle

- The cycle shows all the steps needed to turn atoms into gaseous ions and from gaseous ions into the ionic lattice
- The alternative route to the ionic lattice begins from the enthalpy of formation of the elements in their standard states

Drawing the cycle for sodium chloride

- A good starting point is to draw the elements with their state symbols about a third of the way up the diagram
- This is shown as the left hand side of the equation for the process indicated
- The location is marked by drawing a horizontal bar or line which represents the starting energy level

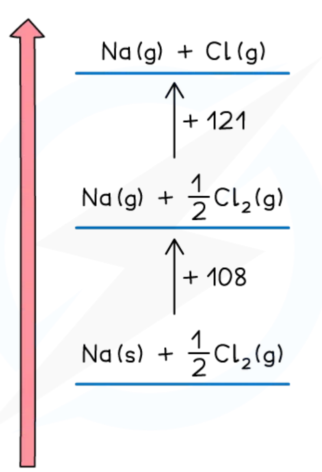
Drawing a Born-Haber cycle- Step 1



Start with your ionic solid

- Next, we need to create the gaseous ions
- This is a two step process of first creating the gaseous atoms and then turning them into ions
- Creating gaseous atoms is a bond breaking process, so arrows must be drawn upwards
- It doesn't matter whether you start with sodium or chlorine
- The enthalpy of atomisation of sodium is
  Na (s) → Na (g) ΔH°_{at} = +108 kJ mol^{-1}
- The enthalpy of atomisation ($\Delta H^{\circ}at$) of chlorine is
  $\frac{1}{2}Cl_2$ (g) → Cl (g) ΔH°_{at} = +121 kJ mol^{-1}
- We can show the products of the process on the horizontal lines and the energy value against a vertical arrow connecting the energy levels

Drawing a Born-Haber cycle- Step 2



Create the gaseous atoms

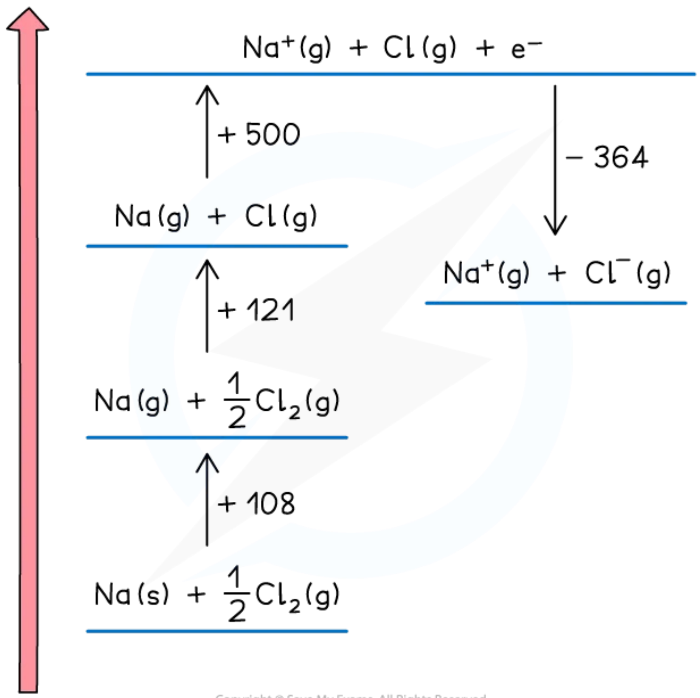
- Now that the ions are created:

- The sodium ion loses an electron, so this energy change is the first ionisation energy (ΔH°_{IE}) for sodium

  $Na (g) \rightarrow Na^{+} (g) + e^{-}$ $\Delta H^{\circ}_{IE} = +500\ kJ\ mol^{-1}$
- The change is endothermic so the direction continues upwards
- The chlorine atom gains an electron, so this is electron affinity (ΔH°_{EA})

  $Cl (g) + e^{-} \rightarrow Cl^{-} (g)$ $\Delta H^{\circ}_{EA} = -364\ kJ\ mol^{-1}$
- The exothermic change means this is downwards
- The change is displaced to the right to make the diagram easier to read

Drawing a Born-Haber cycle- Step 3



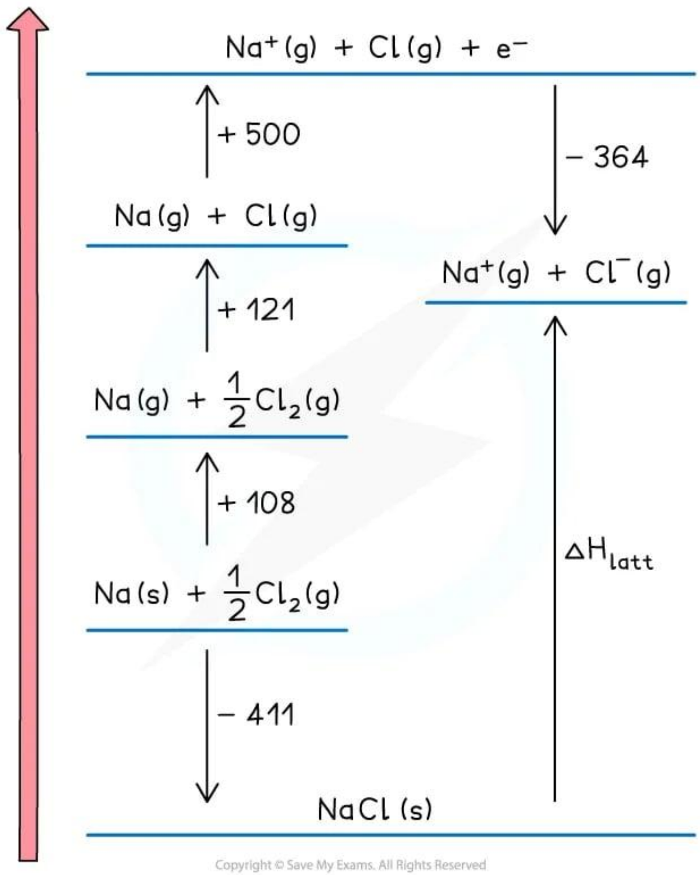
Create the gaseous ions

- The two remaining parts of the cycle can now be completed
- The enthalpy of formation (ΔH°_{f}) of sodium chloride is added at the bottom of the diagram

  $Na(s) + \frac{1}{2}Cl_2 (g) \rightarrow NaCl (s)$ $\Delta H^{\circ}_{f} = -411\ kJ\ mol^{-1}$
- This is an exothermic change for sodium chloride so the arrow points downwards
- Enthalpy of formation can be exothermic or endothermic, so you may need to show it above the elements (and displaced to the right) for a endothermic change
- The final change is lattice enthalpy (ΔH°_{latt}), which is shown as the change from solid to gaseous ions. This means the arrow must point upwards. For sodium chloride, the equation is

  $NaCl (s) \rightarrow Na^{+}(g) + Cl^{-}(g)$ ΔH°_{latt}

Drawing a Born-Haber cycle- Step 4



Complete the cycle

- The cycle is now complete
- The cycle is usually used to calculate the lattice enthalpy of an ionic solid, but can be used to find other enthalpy changes if you are given the lattice enthalpy

Worked Example

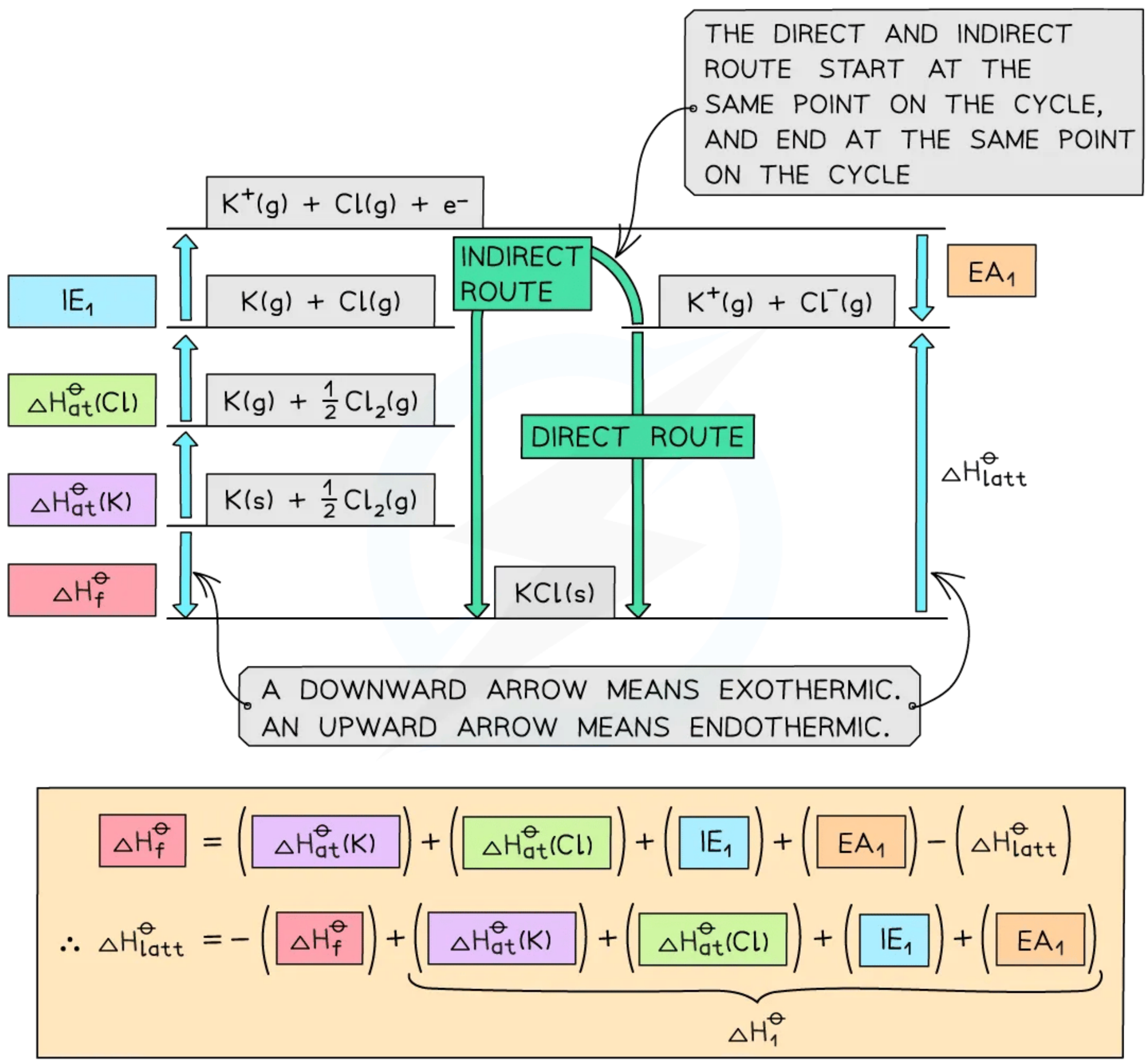
Constructing a Born-Haber cycle for KCl

Construct a Born-Haber Cycle which can be used to calculate the lattice energy of potassium chloride.

Step	Equation	Enthalpy Change
Convert K (s) atoms into K (g) atoms	K (s) → K(g)	Atomisation, ΔH°_{at}
Convert K(g) atoms into K^+ (g) ions	K (g) → K^+ (g) + e^-	First ionisation, IE_1
Convert Cl_2 (g) molecules into Cl (g) atoms	½Cl_2 (g) → Cl (g)	Atomisation, ΔH°_{at}
Convert Cl (g) atoms into Cl^- (g) ions	Cl (g) + e^- → Cl^-(g)	Electron affinity, EA_1

Add up all the values to get ΔH°_1		$\Delta H^\circ 1$
Apply to Hess's law to get ΔH°_{lat}		Lattice enthalpy, ΔH°_{latt}

Answer:



Worked Example

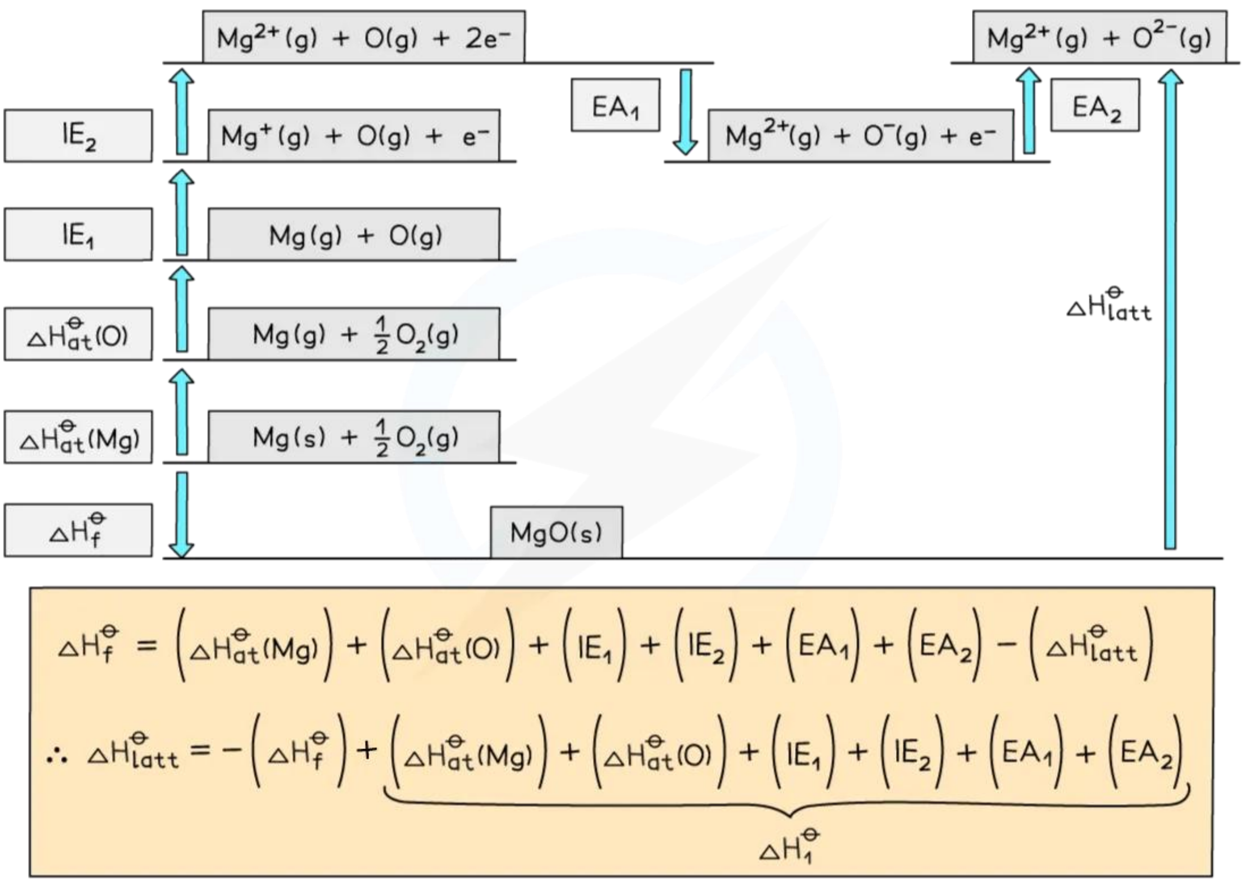
Constructing a Born-Haber cycle for MgO

Construct a Born-Haber Cycle which can be used to calculate the lattice energy of magnesium oxide.

Step	Equation	Enthalpy Change
Convert Mg (s) atoms into Mg (g) atoms	Mg (s) → Mg (g)	Atomisation, ΔH°_{at}

Convert Mg (g) atoms into Mg^+ (g) ions	Mg (g) → Mg+ (g) + e-	First ionisation energy, IE_1
Convert Mg^+ (g) ions into Mg^{2+} (g) ions	Mg+(g) →Mg2+ + e-	Second ionisation energy, IE_2
Convert O_2 (g) molecules into O (g) atoms	½O2 (g) → O(g)	Atomisation, $\Delta H^\ominus_{at}$
Convert O(g) atoms into O^-(g) ions	O (g) + e- → O- (g)	First electron affinity, EA_1
Convert O^-(g) ions into O^{2-}(g) ion	O-(g) + e- →O2- (g)	Second electron affinity, EA_2
Add up all the values to get $\Delta H^\ominus_1$		$\Delta H^\ominus_1$
Apply to Hess's law to get $\Delta H^\ominus_{lat}$		Lattice enthalpy, $\Delta H^\ominus_{latt}$

Answer:



Examiner Tips and Tricks

You will not be asked to drawn an entire Born-Haber cycle from scratch but could be asked to complete a partially drawn one. When constructing Born-Haber cycles, the direction of the changes is important, but the relative size of the steps does not matter so don't worry if the steps don't correspond to the magnitude of the energy changes.
You don't need to show the energy axis in a Born-Haber cycle, but you do need to show the electron(s) in the ionisation step otherwise you might lose marks in an exam.

Born-Haber Cycle Calculations

- Once a Born-Haber cycle has been constructed, it is possible to calculate the lattice enthalpy ($\Delta H^{\ominus}_{lat}$) by applying Hess's law and rearranging:
  $\Delta H^{\ominus}_{f} = \Delta H^{\ominus}_{at} + \Delta H^{\ominus}_{at} + IE + EA - \Delta H^{\ominus}_{lat}$
- If we simplify this into three terms, this makes the equation easier to see:
  - $\Delta H^{\ominus}_{lat}$
  - $\Delta H^{\ominus}_{f}$
  - $\Delta H^{\ominus}_{1}$ (the sum of all of the various enthalpy changes necessary to convert the elements in their standard states to gaseous ions)
- The simplified equation becomes:
  $\Delta H^{\ominus}_{f} = \Delta H^{\ominus}_{1} - \Delta H^{\ominus}_{lat}$
- So, if we rearrange to calculate the lattice enthalpy, the equation becomes
  $\Delta H^{\ominus}_{lat} = - \Delta H^{\ominus}_{f} + \Delta H^{\ominus}_{1}$
- When calculating the $\Delta H^{\ominus}_{lat}$, all other necessary values will be given in the question
- A Born-Haber cycle could be used to calculate any stage in the cycle
  - For example, you could be given the lattice enthalpy and asked to calculate the enthalpy change of formation of the ionic compound
  - The principle would be exactly the same
  - Work out the direct and indirect route of the cycle (the stage that you are being asked to calculate will always be the direct route)
  - Write out the equation in terms of enthalpy changes and rearrange if necessary to calculate the required value
- Remember: sometimes a value may need to be doubled or halved, depending on the ionic solid involved
  - For example, with $MgCl_2$ the value for the first electron affinity of chlorine would need to be doubled in the calculation, because there are two moles of chlorine atoms
  - Therefore, you are adding 2 moles of electrons to 2 moles of chlorine atoms, to form 2 moles of chloride ions, i.e. $2Cl^-$

Worked Example

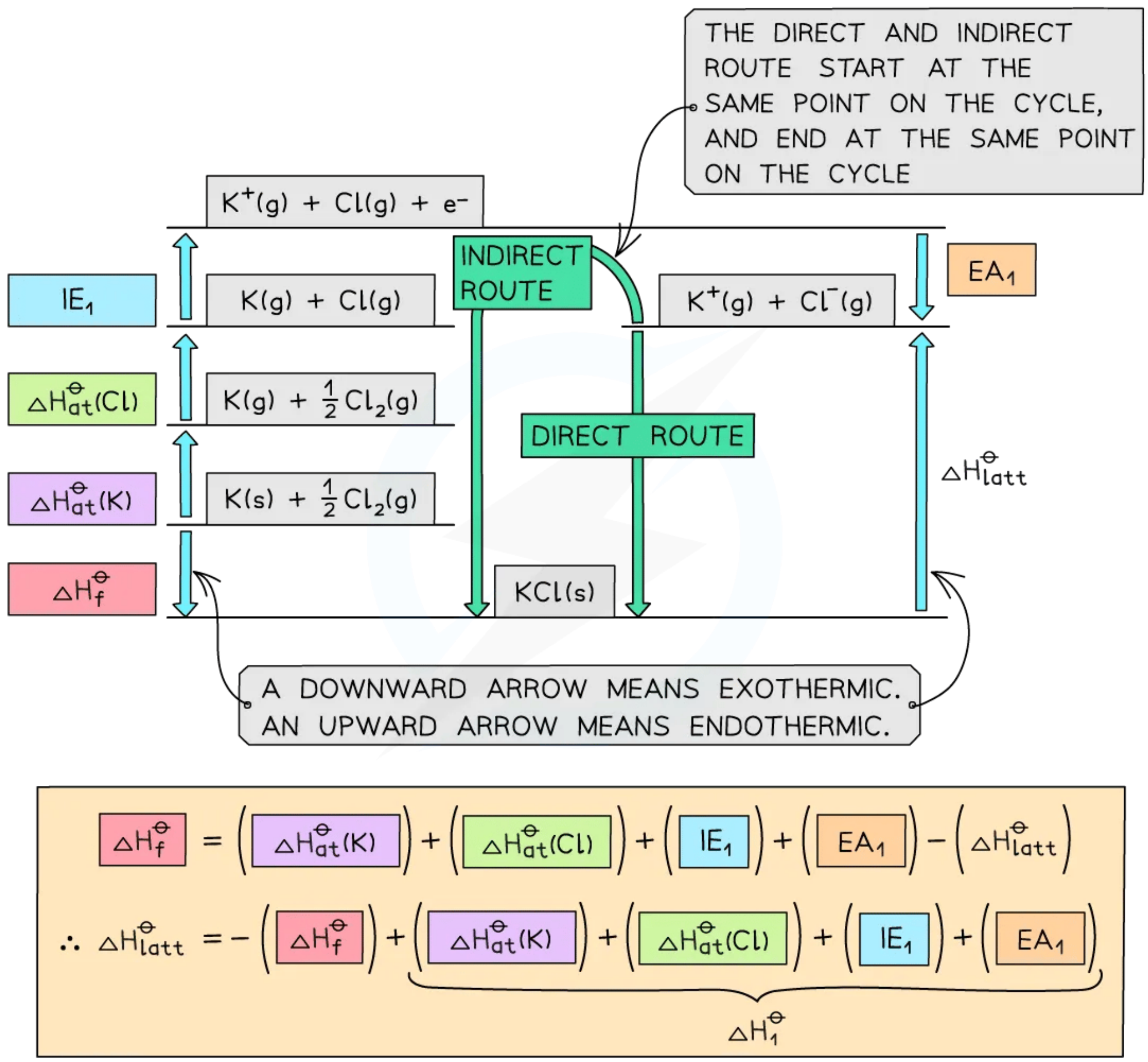
Calculating the lattice enthalpy of KCl
Given the data below, calculate the $\Delta H^{\ominus}_{lat}$ of potassium chloride (KCl).

	$\Delta H^{\ominus}_{at}$ ($kJmol^{-1}$)	IE / EA ($kJmol^{-1}$)

K	+90	+418
Cl	+122	-349
$\Delta H^{\ominus}_f$ (kJmol-1)		
KCl	-437	

Answer:

- Step 1: Construct the Born-Haber cycle



- Step 2: Applying Hess' law, the lattice enthalpy of KCl is:

$\Delta H^{\ominus}_{lat} = -\Delta H^{\ominus}_f + \Delta H^{\ominus}_1$

$\Delta H^{\ominus}_{lat} = -\Delta H^{\ominus}_f + [(\Delta H^{\ominus}_{at}\ K) + (\Delta H^{\ominus}_{at}\ Cl) + (IE_1\ K) + (EA_1\ Cl)]$

- Step 3: Substitute in the numbers:

$\Delta H^{\ominus}_{lat} = -(-437) + [(+90) + (+122) + (+418) + (-349)] = 718\ kJ\ mol^{-1}$

Worked Example

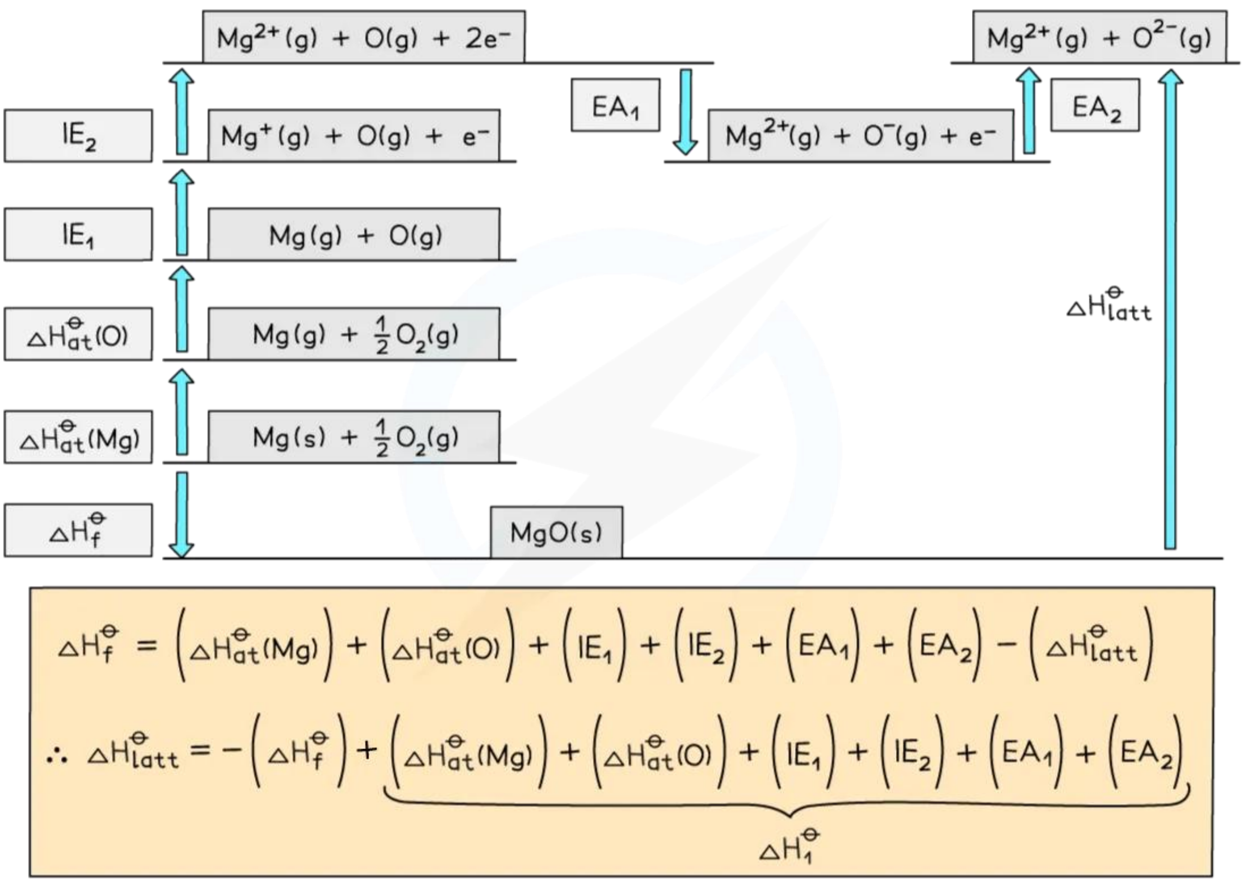
Calculating the lattice enthalpy of MgO

Given the data below, calculate the of ΔH⊖lat magnesium oxide of magnesium oxide (MgO)

	$\Delta H^{\ominus}_{at}$ ($kJmol^{-1}$)	IE_1 / EA_1($kJmol^{-1}$)	IE_1 / EA_1($kJmol^{-1}$)
Mg	+148	+736	+1450
O	+248	-142	+770
		$\Delta H^{\ominus}_{f}$ ($kJmol^{-1}$)	
MgO	-602		

Answer:

- Step 1: Construct the Born-Haber cycle



- Step 2: Applying Hess' law, the lattice enthalpy of MgO is:

$\Delta H^{\ominus}_{lat} = -\Delta H^{\ominus}_{f} + \Delta H^{\ominus}_{1}$

$\Delta H^{\ominus}_{lat} = -\Delta H^{\ominus}_{f} + [(\Delta H^{\ominus}_{at}\ Mg) + (\Delta H^{\ominus}_{at}\ O) + (IE_1\ Mg) + (IE_2\ Mg) + (EA_1\ O) + (EA_2\ O)]$

- Step 3: Substitute in the numbers:

$\Delta H^{\ominus}_{lat} = -(-602) + [(+148) + (+248) + (+736) + (+1450) + (-142) + (+770)]$

$= 3812\ kJ\ mol^{-1}$