Unit 5, Lesson 02: Predicting the Direction of a Reversible Reaction

When the driving forces behind a reaction are acting in opposite directions, how can we predict whether or not a reaction will occur? There is an equation called the "Gibb's Free Energy" (ΔG) equation and it looks at the overall balance between the changes in enthalpy (ΔH) and changes in entropy (ΔS):



 ΔG (Gibb's Free Energy) allows us to calculate the overall amount of energy (the free or useful amount of energy) released or absorbed by a system during a chemical reaction, at a stated temperature. Note that temperature is multiplied by the entropy term only. Entropy <u>is</u> affected by temperature, while enthalpy is not.

eg. For the following reaction at 25°C (298 K): N₂ (g) + 3 H₂ (g) \rightarrow 2 NH₃ (g) Δ H = -91.8 kJ

- The reaction is exothermic so enthalpy decreases (ΔH is negative) which will favour the products. The drive to lower energy will push the reactant forward.
- There are four moles of gas on the reactant side of the equation, and only two moles of gas as products, so entropy decreases, which does not favour the products. The drive to maximum entropy favours the reverse reaction. This will tend to push the reaction backward.
- So, at $25^{\circ}C(25^{\circ}C + 273) = 298$ K, how do we know which driving force will predominate?
- To find out if the reaction will proceed, we need to calculate the value of ΔG , the free energy change, using the equation $\Delta G = \Delta H T \Delta S$. If ΔG is negative, the forward reaction will occur.

Given: $\Delta H = -91.8 \text{ kJ}$ (exothermic, energy released)

 $\Delta S = -197 \text{ J/K}$ (entropy decreases, convert to kJ/K by dividing by 1000)

 $T = 25^{\circ}C \text{ or } 298 \text{ K}$

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

= -91.8 kJ - (298 K x -0.197 kJ/K) the K will cancel out of the T Δ S term

= -91.8 kJ + 58.7 kJ

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= -33.1 \text{ kJ}
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The overall value of ΔG is negative. This tells us that the forward reaction will be favoured overall, and that the reaction will be spontaneous at a temperature of 298K.

Now, what happens at a higher temperature, say 700K? This will change the T Δ S term:

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\Delta G = \Delta H - T \Delta S
= -91.8 kJ - (700 K x -0.197 kJ/K)
= -91.8 kJ + 137.9 kJ
= 46.1 kJ
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At this higher temperature, the entropy of the reactants is so much greater than the entropy of the products, that the reaction will not proceed (is not spontaneous) at 700K.

We will not be doing calculations to find ΔS (you can look forward to that at University). However, if you are given the values for ΔH , ΔS and temperature, you are expected to be able to calculate the value for ΔG , and then interpret what this value means in terms of the reaction proceeding:

- a) If ΔG is negative:
- the reaction releases a large amount of free energy
- the reaction will proceed to the right (favours products)
- the reaction is said to be spontaneous. This means that the system does not require the addition of energy, once the activation energy has been supplied
- b) If ΔG is positive:
- the reaction absorbs a large amount of free energy
- the reaction will not proceed to the right. The reaction favours the reactants
- the reaction is non-spontaneous at this temperature
- c) If ΔG is zero:
- the forward and reverse reactions are equally favoured
- there is no net free energy change
- the system is in equilibrium (what does this mean? we'll see in the next lesson)

| TABLE 20.1 | | Criteria for Spontaneous Change: $\Delta G = \Delta H - T \Delta S$ | | | |
|------------|---------------|---|--|----------------------------|--|
| Case | ΔH | ΔS | ΔG | Result | Example |
| 1 | : | + | <u></u> | spontaneous at all temp | $2 N_2 O(g) \longrightarrow 2 N_2(g) + O_2(g)$ |
| 2 | <u></u> | <u> 11</u> 1 | $\begin{pmatrix} -\\ + \end{pmatrix}$ | spontaneous at low temp | $H_2O(1) \longrightarrow H_2O(s)$ |
| 3 | + | + | $\left\{ egin{array}{c} + \\ - \end{array} ight.$ | nonspontaneous at low temp | $2 \operatorname{NH}_3(g) \longrightarrow \operatorname{N}_2(g) + 3 \operatorname{H}_2(g)$ |
| 4 | + | <u>1800.</u> | + | nonspontaneous at all temp | $3 O_2(g) \longrightarrow 2 O_3(g)$ |