

Quiz 3.3 - Gibbs Energy and T

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The Equilibrium Temperature

Consider the Haber-Bosch process: $3 \text{H}_2(\text{g}) + \text{N}_2(\text{g}) \rightleftharpoons 2 \text{NH}_3(\text{g})$ At 298 K this reaction has $\Delta G^\ominus = -32.90 \frac{\text{kJ}}{\text{mol}}$, $\Delta H^\ominus = -92.22 \frac{\text{kJ}}{\text{mol}}$, and $\Delta S^\ominus = -198.76 \frac{\text{J}}{\text{mol K}}$ In CHEM 1220 you learned that $\Delta G = \Delta H - T\Delta S$, and used this formula to calculate the equilibrium temperature: $T = \frac{\Delta H}{\Delta S}$. Use this formula to find the equilibrium temperature.

$$T = \frac{-92.22 \frac{\text{kJ}}{\text{mol}}}{-0.19876 \frac{\text{kJ}}{\text{mol K}}} = 464 \text{ K}$$

That formula relies on the assumption that ΔH and ΔS are both independent of temperature, which is only a good approximation over very small temperature ranges. Use Kirchoff's law to find ΔH and use $\Delta S(T_2) = \Delta S(T_1) + \int_{T_1}^{T_2} \frac{\Delta C_p}{T} dT$ to find ΔS at the equilibrium temperature you calculated above

$$\Delta H(464) = -92.22 \frac{\text{kJ}}{\text{mol}} - 0.04988 \frac{\text{kJ}}{\text{mol K}} \cdot 166 \text{ K} = -100.5 \frac{\text{kJ}}{\text{mol}}$$

$$\Delta S(464) = -198.76 \frac{\text{J}}{\text{mol K}} - 49.88 \frac{\text{J}}{\text{mol K}} \cdot \ln\left(\frac{464}{298}\right) = -220.8 \frac{\text{J}}{\text{mol K}}$$

Use these values of ΔH and ΔS to find ΔG at the equilibrium temperature you calculated above. Is the system really at equilibrium?

$$\Delta G = -100.5 \frac{\text{kJ}}{\text{mol}} - 464 \text{ K} \cdot -0.2208 \frac{\text{kJ}}{\text{mol K}} = +1.95 \frac{\text{kJ}}{\text{mol}}$$

No, $\Delta G \neq 0$ Find the true equilibrium temperature using the Gibbs-Helmholtz equation: $\left(\frac{d(\Delta G/T)}{dT}\right)_p = -\frac{\Delta H}{T^2}$

The answer is 454.4 K, but this is a bad question so please don't feel like you need to solve it.

Find ΔH and ΔS at that temperature, and confirm that the system is at equilibrium at that temperature