Quiz 6.1 – Equilibrium

Name: Key

The Equilibrium Constant

Consider the reaction below:

1 mol ... 2 moles

$PCl_5(g) \rightleftharpoons PCl_3(g) + Cl_2(g)$ $\qquad K_C(25°C) = 0.0160$

○ Find the value of K_p for this reaction at $25°C$

Note which version of R we use

$K_p = K_c \cdot (RT)^{\Delta n}$ $\qquad K_p = 0.0160 \cdot \left(0.08314 \frac{L \cdot bar}{mol \cdot K} \cdot 298\,K\right) = 0.396$

○ Find the value of $\Delta G^{\ominus}_{rxn}$ for this reaction at $25°C$

(*Note that the standard state for all chemical species in this reaction is a gas at 1 bar*)

$\Delta G^\circ = -RT \ln K = -0.008314 \frac{kJ}{mol \cdot K} \cdot 298\,K \cdot \ln(0.396) = 2.30 \frac{kJ}{mol}$

○ Find the value of ΔG_{rxn} when $p_{PCl_5} = 0.53\ bar$, $p_{PCl_3} = 0.22\ bar$, and $p_{Cl_2} = 0.47\ bar$

$Q = \frac{0.22\ bar \cdot 0.47\ bar}{0.53\ bar} = 0.195$

$\Delta G = \Delta G^\circ + RT \ln Q = 2.30 \frac{kJ}{mol} + 0.008314 \frac{kJ}{mol \cdot K} \cdot 298\,K \cdot \ln(0.195) = -1.75 \frac{kJ}{mol}$

Le Châtelier's Principle

Syngas, a mixture of carbon monoxide and hydrogen gas, can be produced by reacting methane with water in the reaction below:

2 moles ... 4 moles

heat + $CH_4(g) + H_2O(g) \rightleftharpoons CO(g) + 3\,H_2(g)$ $\qquad \Delta_{rxn}H^{\ominus}(273\ K) = 206.13\ ^{kJ}/_{mol}$ endothermic

You are a chemical engineer designing a new syngas production plant, and you want to maximize the amount of syngas produced (maximize ξ) at equilibrium.*

○ Should you run the reaction at high or low temperature?

High T

○ Should you run the reaction with high partial pressures or low partial pressures?

Low pressures

*Really, chemical engineers consider far more diverse and complex factors when designing plants

The van't Hoff Equation

Consider the reaction below:

$$H_2(g) + Br_2(g) \rightleftharpoons 2\,HBr(g)$$

For all these problems use $\ln\left(\frac{K_2}{K_1}\right) = -\frac{\Delta H^\circ}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)$

This reaction is carried out at two temperatures while monitoring equilibrium composition. At 25°C, the reaction has $K = 62.5$, and at 175°C the reaction has $K = 0.00343$.
Use these data to find $\Delta H^{\ominus}_{rxn}$ for this reaction.

$$\ln\left(\frac{0.00343}{62.5}\right) = \frac{-\Delta H^\circ}{0.008314 \frac{kJ}{mol\,K}}\left(\frac{1}{448\,K} - \frac{1}{298\,K}\right) \rightarrow \Delta H^\circ = -72.6\ \frac{kJ}{mol}$$

What is the value of K at $-15°C$?

$$\ln\left(\frac{K_2}{62.5}\right) = \frac{+72{,}600\ \frac{J}{mol}}{8.314\ \frac{J}{mol \cdot K}}\left(\frac{1}{258\,K} - \frac{1}{298\,K}\right) \rightarrow K_2 = 5870$$

At what temperature is $K = 1.00$?

$$\ln\left(\frac{1.00}{62.5}\right) = \frac{72{,}600\ \frac{J}{mol}}{8.314\ \frac{J}{mol \cdot K}}\left(\frac{1}{T_2} - \frac{1}{298\,K}\right) \rightarrow T_2 = 347\ K\ (74°C)$$

At right, draw a rough van't Hoff plot for this reaction, including:

- Equation for the best fit line $y = 8731x - 25.2$
- Relationship for the slope $\text{Slope} = -\frac{\Delta H}{R}$
- K in the high temperature limit $1.14 \cdot 10^{-11}$
- K in the low temperature limit ∞