

Problem 3. (10 points total)

Consider a hypothetical reaction: $A \rightleftharpoons B$ with the $\Delta G^{\circ} = -5 \text{ kJ/mol}$ for the forward reaction. The molar concentrations at the beginning of the reaction were $[A] = 12 \text{ mM}$, $[B] = 0$.

at 25°C

(a) (4 pts) One hour later the concentrations were $[A] = 10 \text{ mM}$, $[B] = 2 \text{ mM}$. Calculate the ΔG of the reaction at this point. Has the reaction reached the equilibrium?

$$\Delta G = \Delta G^{\circ} + RT \ln \frac{[B]}{[A]} = -5 \frac{\text{kJ}}{\text{mol}} + 8.315 \frac{\text{J}}{\text{mol}\cdot\text{K}} \cdot 298 \text{ K} \cdot \ln \frac{2}{10}$$

$$= -8.988 \frac{\text{kJ}}{\text{mol}}$$

$\Delta G \neq 0$, hence the reaction has not reached the equilibrium

(b) (6 pts) Calculate the molar concentrations of A and B at the equilibrium (show the calculations).

$$K_{\text{eq}} = \frac{[B]_{\text{eq}}}{[A]_{\text{eq}}} = e^{-\Delta G^{\circ}/RT} = 7.52$$

To determine $[B]_{\text{eq}}$ and $[A]_{\text{eq}}$ separately, use "matter conservation" law:

$$[A]_{\text{eq}} + [B]_{\text{eq}} = 12 \text{ mM}.$$

Let $[A]_{\text{eq}} = x$; then $[B]_{\text{eq}} = 7.52x$, and we have $(x + 7.52x) = 12 \text{ mM}$.

$$\text{We get } [A]_{\text{eq}} = 1.4 \text{ mM}$$

$$[B]_{\text{eq}} = 10.6 \text{ mM}$$