Problem 5-01 Reaction Gibbs energy and direction of chemical reaction

The standard reaction Gibbs energy of the reaction

$$\textbf{2-P-glycerate}^{3-} = \textbf{2-P-enolpyruvate}^{3-} + \textbf{H}_2\textbf{O}\ (\ell)$$

at the temperature of 37.3 °C is $\Delta_r G^{\ominus} = -2.68$ kJ mol^{-1} (standard states: infinite dilution, $c^{st} = 1$ mol dm^{-3}, for solutes, pure substance at given temperature and pressure). Find out if this reaction is exergonic or endergonic at standard conditions. Calculate the reaction Gibbs energy of the reaction in the instant when the concentrations of components are

(a) c(2-P-glycerate^{3-}) = 0.015 mol dm^{-3} and c(2-P-enolpyruvate^{3-}) = 0.032 mol dm^{-3}

(b) c(2-P-glycerate^{3-}) = $5\cdot10^{-2}$ mol dm^{-3} and c(2-P-enolpyruvate^{3-}) = $7.5\cdot10^{-4}$ mol cm^{-3}

Decide if the reaction will go to the products or to the reactants. Assume that all activity coefficients are equal to one.

[$\Delta_r G^{\ominus} < 0$ – exergonic; (a) $\Delta_r G = -724.3$ J mol^{-1} – the reaction goes to products;
(b) $\Delta_r G = +3940.3$ J mol^{-1} – the reaction goes to reactants]

Solution:

2-P-glycerát^{3-} ≡ G
2-P-enolpyruvát^{3-} ≡ E
T = 37.3 + 273.15 = 310.45 K

$\Delta_r G^{\ominus} = -2.68$ kJ mol^{-1} < 0 , reaction is exergonic

$$\Delta_r G = \Delta_r G^{\ominus} + \boldsymbol{R}T \ln \frac{a_E \cdot a_{H2O}}{a_G}$$

$$a_i = \gamma_i \cdot \frac{c_i}{c^{st}} \quad , \quad \gamma_i = 1 \quad , \quad a_{H2O} = 1$$

(a) $c_G = 0.015$ mol dm^{-3}
$c_E = 0.032$ mol dm^{-3}

$$\Delta_r G = -2680 + 8.314 \cdot 310.45 \cdot \ln \frac{0.032}{0.015} = -2680 + 1955.65$$

$\Delta_r G = -724.35$ J mol^{-1} < 0 , reaction runs towards products

(b) $c_G = 0.05$ mol dm^{-3}
$c_E = 6.5\cdot10^{-4}$ mol cm^{-3} = 0,65 mol dm^{-3}

$$\Delta_r G = -2680 + 8.314 \cdot 310.45 \cdot \ln \frac{0.65}{0.05} = -2680 + 6620.34$$

$\Delta_r G = +3940.34$ J mol^{-1} > 0 , reaction runs towards reactants