Problem 5-02 Reaction Gibbs energy and direction of chemical reaction

The reaction

glucose-1-phosphate = glucose-6-phosphate,

catalyzed by phosphoglucomutase, is a part of carbohydrate metabolism. The equilibrium constant at 25 °C, K = 18.8 is valid for the standard state infinite dilution, c^{st} = 1 mol dm^{-3}. Find out what will arise in the mixture containing both components in concentrations 5.55 mmol dm^{-3} of glucose-1-phosphate and 0.555 mol dm^{-3} of glucose-6-phosphate: 1-phosphate or 6-phosphate? What will be the composition of the equilibrium mixture? Assume that all activity coefficients are equal to one.

[$\Delta_r G$ = 4.14 kJ mol^{-1} > 0 , glucose-1-phosphate is formed,
in equilibrium: 94.95 mol. % of glucose-6-phosphate]

Solution:

glucose-1-phosphate ≡ G1F
glucose-6-phosphate ≡ G6F

T = 25 + 273.15 = 298.15 K
K = 18.8
$\Delta_r G^{\ominus} = -\boldsymbol{R}T \ln K = -8.314 \cdot 298.15 \cdot \ln 18.8 = -7272.5$ J mol^{-1}

$$\Delta_r G = \Delta_r G^{\ominus} + \boldsymbol{R}T \ln \frac{(a_{G6F})_0}{(a_{G1F})_0}$$

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

$(c_{G1F})_0$ = 5.55 mmol dm^{-3} = 0.00555 mol dm^{-3}
$(c_{G6F})_0$ = 0.555 mol dm^{-3}

$$\Delta_r G = -7272.5 + 8.314 \cdot 298.15 \cdot \ln \frac{0.555}{0.00555} = -7272.5 + 11415.384 = 4142.884 \text{ J mol}^{-1}$$

$\Delta_r G$ = 4.14 kJ mol^{-1} > 0 , glucose-1-phosphate is formed:

glucose-6- phosphate → glucose-1- phosphate

Equilibrium conversion: $x_{equil} = \xi_{equil} / V$(mol dm^{-3})

$(c_{G6F})_r = (c_{G6F})_0 - x_{equil} = 0.555 - x_{equil}$
$(c_{G1F})_r = (c_{G1F})_0 + x_{equil} = 0.00555 + x_{equil}$

$$K = \frac{(c_{G6F})_{equil}}{(c_{G1F})_{equil}} = \frac{(c_{G6F})_0 - x_{equil}}{(c_{G1F})_0 + x_{equil}}$$

$$18.8 = \frac{0.555 - x_{equil}}{0.00555 + x_{equil}}$$

$0.10434 + 18.8\, x_{equil} = 0.555 - x_{equil}$

$$x_{equil} = \frac{0.555 - 0.10434}{18.8 + 1} = 0{,}02276$$

$(c_{G6F})_{equil}$ = 0.555 – 0.02276 = 0.53224 mol dm^{-3} .....$100 \cdot \frac{0.53224}{0.56055}$ = 94.95 mol.%

$(c_{G1F})_{equil}$ = 0.00555 + 0.02276 = 0.02831 mol dm^{-3} .....$100 \cdot \frac{0.02831}{0.56055}$ = 5.05 mol.%

Σc = 0.53224 + 0.02831 = 0.56055 mol dm^{-3}