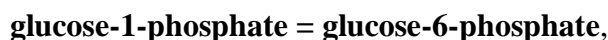


Problem 5-02 Reaction Gibbs energy and direction of chemical reaction

The reaction



catalyzed by phosphoglucumutase, is a part of carbohydrate metabolism. The equilibrium constant at 25°C, $K = 18.8$ is valid for the standard state infinite dilution, $c^{\text{st}} = 1 \text{ mol dm}^{-3}$. Find out what will arise in the mixture containing both components in concentrations $5.55 \text{ mmol dm}^{-3}$ of glucose-1-phosphate and $0.555 \text{ mol dm}^{-3}$ 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.

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

Solution:

glucose-1-phosphate \equiv G1F

glucose-6-phosphate \equiv G6F

$$T = 25 + 273.15 = 298.15 \text{ K}$$

$$K = 18.8$$

$$\Delta_r G^\ominus = -RT \ln K = -8.314 \cdot 298.15 \cdot \ln 18.8 = -7272.5 \text{ J mol}^{-1}$$

$$\Delta_r G = \Delta_r G^\ominus + RT \ln \frac{(a_{\text{G6F}})_0}{(a_{\text{G1F}})_0}$$

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

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

$$(c_{\text{G6F}})_0 = 0.555 \text{ mol dm}^{-3}$$

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

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

glucose-6- phosphate \rightarrow glucose-1- phosphate

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

$$(c_{\text{G6F}})_r = (c_{\text{G6F}})_0 - x_{\text{equil}} = 0.555 - x_{\text{equil}}$$

$$(c_{\text{G1F}})_r = (c_{\text{G1F}})_0 + x_{\text{equil}} = 0.00555 + x_{\text{equil}}$$

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

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

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

$$x_{\text{equil}} = \frac{0.555 - 0.10434}{18.8 + 1} = 0.02276$$

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

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

$$\Sigma c = 0.53224 + 0.02831 = 0.56055 \text{ mol dm}^{-3}$$