Key

Discussion Worksheet: Quantitative Thermodynamics

Skill 1: Standard free energy and equilibrium

Problem 1. The reaction of fructose-1,6-bisphosphate to form dihydroxyacetone phosphate and glyceraldehyde-3-phosphate was allowed to reach equilibrium. The concentrations of DHAP and GA-3-P were both found to be 2.2×10^{-4} M. If the standard free energy of this reaction is +23.8 kJ/mol, what is the equilibrium concentration of fructose-1,6-bisphosphate in this reaction?

First, write the rxn: F-1,6-bP $\rightleftharpoons$ DHAP + GA-3-P

Second, solve for K_{eq}

$\Delta G^{o'} = -RT \ln K_{eq}$ $\quad 23{,}800 \frac{J}{mol} = -8.314 \frac{J}{mol\,K}(298) \ln K_{eq}$

$K_{eq} = 6.70 \times 10^{-5}$

Third, determine [F16bP]

$K_{eq} = \frac{[DHAP][GAP]}{[F16bP]}$ $\quad 6.7 \times 10^{-5} = \frac{[2.2 \times 10^{-4}][2.2 \times 10^{-4}]}{[F16bP]}$

$[F16bP] = 7.2 \times 10^{-4}\ M$

Skill 2: Phosphoryl transfer and Hess' Law

Problem 2. Calculate the standard free energy of the phosphorylation of creatine using ATP. Is this reaction spontaneous or not under standard conditions?

First, write the equation of creatine phosphorylation

creatine + ATP $\rightleftharpoons$ creatine phosphate + ADP

Second, write 2 half-reactions in terms of hydrolysis:

creatine + (P) $\rightarrow$ creatine phosphate $\quad \Delta G^{o'} = +43.1 \frac{kJ}{mol}$

ATP $\rightarrow$ ADP + (P) $\quad \Delta G^{o'} = -30.5 \frac{kJ}{mol}$

Third: Add $\Delta G^{o'}$ from table 15.1 using Hess' Law

$\Delta G^{o'}$ of creatine phosphorylation = $+12.6 \frac{kJ}{mol}$ not spontaneous

Skill 3: Free energy vs. Standard Free energy

not ΔG° ↓

Problem 3: Refer to the text solve problems 15.30 and 15.31.

Problem 15.30 - error in wording: should say, "whereas $\Delta G'$ in the cell is -1.3 kJ/mol..."

Part 1: ΔG° is used to calculate K_{eq} as in problem 1

$$K_{eq} = \frac{[DHAP][GA\text{-}3\text{-}P]}{[F16bP]} = 6.7 \times 10^{-5}$$

Part 2: under cellular conditions

$$\Delta G' = \Delta G^{\circ\prime} + RT \ln \frac{[R]}{[P]}$$

$$-1300 \frac{J}{mol} = +23,800 \frac{J}{mol} + 8.314 \frac{J}{mol\,K} (298k) \ln \frac{[DHAP][GA\text{-}3P]}{[F16bP]}$$

$$\frac{[DHAP][GA\text{-}3P]}{[F16bP]} = 3.9 \times 10^{-5}$$

Part 3: The rxn is spontaneous under cellular conditions, because under cellular conditions, the ratio of P/R is below equilibrium, so the rxn will spontaneously produce more product.

Problem 15.31: see solution in book