7.2) The concentration of fructose 6-phosphate (F6P) and fructose 1,6-biphosphate (F16bP), ATP, and ADP in muscle tissue were measured as 0.089, 0.012, 12.0, and 1.2 mmol/L. For the reaction F6P(aq) + ATP(aq) → F16bP(aq) + ADP(aq) at 37°C, the standard Gibbs energy (at pH=7) is −18.3 kJ/mol. (a) Calculate the reaction quotient and the reaction Gibbs energy for the reaction in the muscle tissue environment. (b) Is the reaction spontaneous?

a) For the reaction as written,

\[ Q = \frac{[F16bP][ADP]}{[F6P][ATP]} = \frac{(0.012)(1.2)}{(0.089)(12.0)} = 0.01348 \equiv 0.013 \]

\[ \Delta G_r = \Delta G_r^o + RT \ln Q \]

\[ = -18.3 + (8.31451 \times 10^{-3})(310) \ln(0.01348) \]

\[ = -29.4 \text{ kJ/mol} \]

b) Yes, it is spontaneous since \( \Delta G_r < 0 \)

7.3) The standard Gibbs energy of formation of NH3(g) is −16.5 kJ/mol at 298 K.

What is the reaction Gibbs energy when the partial pressures of the N2, H2, and NH3 (treated as perfect gases) are 3.0 bar, 1.0 bar, and 4.0 bar, respectively?

What is the spontaneous direction of the reaction in this case?

The formation reaction is (per mole NH3): \( \frac{1}{2}N_2 + \frac{3}{2}H_2 \rightarrow NH_3 \) and \( \Delta G_f^o = \Delta G_r^o \)

\[ \Delta G_r = \Delta G_r^o + RT \ln \frac{P_{NH_3}}{\left( P_{N_2} \right)^{1/2} \left( P_{H_2} \right)^{3/2}} \]

\[ = -16.5 + (298)(8.31451 \times 10^{-3}) \ln \frac{4.0}{\left( 3.0 \right)^{1/2} \left( 1.0 \right)^{3/2}} \]

\[ = -14.4 \text{ kJ/mol} \]

The spontaneous direction is towards products.
7.6) The equilibrium constant for the reaction \( A + B \rightleftharpoons 2C \) is reported as \( 3.4 \times 10^4 \).

What would it be for the reaction written as

(a) \( 2A + 2B \rightleftharpoons 4C \), (b) \( \frac{1}{2}A + \frac{1}{2}B \rightleftharpoons C \)

For the original reaction, \( K = \frac{[C]^2}{[A][B]} \), and multiplying the reaction by a constant raises the equilibrium constant by that power:

(a) \( K' = \frac{[C]^4}{[A]^2[B]^2} = (K)^2 = 1.2 \times 10^9 \)

(b) \( \sqrt{K} = 1.8 \times 10^2 \)

7.7) The equilibrium constant for the isomerization of \( cis \)-2-butene to \( trans \)-2-butene is \( K = 2.07 \) at 400 K. Calculate the standard reaction Gibbs energy for the isomerization.

\[
\Delta G_r^o = -RT \ln K = -(8.31451)(400) \ln(2.07) = 2.42 \times 10^3 \text{ J} / \text{mol}
\]

\[= -2.42 \text{ kJ} / \text{mol} \]
7.9) One biochemical reaction has a standard Gibbs energy of $-200 \text{ kJ/mol}$ and a second biochemical reaction has a standard Gibbs energy of $-100 \text{ kJ/mol}$. What is the ratio of their equilibrium constants at 310 K?

For each reaction, $\Delta G^o_r = -RT \ln K$:

$$\frac{-100}{-200} = \frac{\ln K_2}{\ln K_1}$$

$$\frac{1}{2} = \frac{\ln K_2}{\ln K_1}$$

$$\frac{1}{2} \ln K_1 = \ln K_2$$

$$\ln K_1^{\frac{1}{2}} = \ln K_2$$

$$K_2 = K_1^{\frac{1}{2}}$$

7.16) Use the information in Appendix 1 to estimate the temperature at which (a) CaCO$_3$ decomposes spontaneously and (b) CuSO$_4$ • 5H$_2$O undergoes dehydration.

Using the relation $\Delta G^o = \Delta H^o - T \Delta S^o$, the breakeven point in the spontaneity of a process is when $\Delta G^o = 0$. If we assume $\Delta H^o$ and $\Delta S^o$ are independent of temperature, the temperature at which this occurs is obtained from $T = \frac{\Delta H^o}{\Delta S^o}$. In the following the $\Delta H^o_r$’s are obtained from $\Delta H^o_f$ data and the $\Delta S^o_r$ are obtained from standard molar entropies, $S^o_m$.

a) for CaCO$_3$ → CaO + O$_2$

$$\Delta H^o_r = -635.1 + (-393.5) - (-1206.9) = 178.3 \text{ kJ/mol}$$

$$\Delta S^o_r = 39.75 + 213.74 - 92.9 = 160.6 \text{ J K}^{-1} \text{ mol}^{-1}$$

$$T = \frac{178.3 \times 10^3}{160.6} = 1110 \text{ K}$$
b) for CuSO$_4$ • 5H$_2$O(s) $\rightarrow$ CuSO$_4$(s) + 5H$_2$O(g)

$$\Delta H^0_r = (-771.36) + 5(-241.82) - (-2279.7) = 299.24 \text{ kJ/mol}$$

$$\Delta S^0_r = (109) + 5(188.83) - (300.4) = 752.75 \text{ J K}^{-1} \text{ mol}^{-1}$$

$$T = \frac{299.24 \times 10^3}{752.75} = 398 \text{ K}$$

7.23) Could the synthesis of ammonia be used as the basis of a fuel cell? What is the maximum electrical energy output for the consumption of 100 g of nitrogen?

The synthesis of ammonia could be used as a fuel cell since it is a spontaneous reaction. Remembering that the maximum amount of non-expansion work (e.g., electrical work) is given by $\Delta G$, for 100 g of N$_2$:

For the reaction, N$_2$ + 3H$_2$ $\rightarrow$ 2NH$_3$,

$$\Delta G_r = 2(-16.45) - (0) - 3(0) = -32.9 \text{ kJ/mol} \quad \text{(using } \Delta G_f \text{'s)}$$

$$100 \text{ g N}_2 \times \frac{1 \text{ mol}}{28.013 \text{ g}} = 3.570 \text{ mol}$$

$$3.570 \text{ mol N}_2 \times 32.9 \frac{\text{kJ}}{\text{mol N}_2} = 117.4 \text{ kJ}$$

7.34) The equilibrium constant of the reaction 2C$_3$H$_6$(g) $\rightleftharpoons$ C$_2$H$_4$(g) + C$_4$H$_8$(g) is found to fit the expression (T in kelvin)

$$\ln K = -1.04 - \frac{1088}{T} + \frac{1.51 \times 10^5}{T^2}$$

between 300 K and 600 K. Calculate the standard reaction enthalpy and standard reaction entropy at 400 K. (Hint: Begin by calculating $\ln K$ at 390 K and 410 K; then use eqn. 7.14.)

At 390 K, $\ln K = -1.04 - \frac{1088}{390} + \frac{1.51 \times 10^5}{390^2} = -2.83698$
At 410 K, \( \ln K' = -1.04 - \frac{1088}{410} + \frac{1.51 \times 10^5}{410^2} = -2.79538 \)

the van’t Hoff equation yields: \( \ln K' - \ln K = \frac{\Delta H_f^o}{R} \left( \frac{1}{T_1} - \frac{1}{T_2} \right) \)

re-arranging for the enthalpy and substituting,

\[
\Delta H_f^o = \frac{R(-2.79538 + 2.83698)}{\left( \frac{1}{390} - \frac{1}{410} \right)} = 2.765 \text{ kJ / mol}
\]

At 400 K, the equation above for the T dependence of \( \ln K \) yields \( \ln K = -2.81625 \) and \( \Delta G_f^o = -RT \ln K = -(8.31451 \times 10^{-3})(400)(-2.81625) = 9.37 \text{ kJ / mol} \)

Finally, \( \Delta S_f^o = \frac{\Delta H_f^o - \Delta G_f^o}{T} = -16.5 \text{ J K}^{-1} \text{ mol}^{-1} \)

7.39) In a gas-phase equilibrium mixture of SbCl\(_5\), SbCl\(_3\), and Cl\(_2\) at 500 K,

\( p_{SbCl_5} = 0.15 \text{ bar}, p_{SbCl_3} = 0.20 \text{ bar}. \) Calculate the equilibrium partial pressure of Cl\(_2\) given that \( K = 3.5 \times 10^{-4} \) for the reaction \( SbCl_5(g) \rightleftharpoons SbCl_3(g) + Cl_2(g) \).

\[
K = \frac{p_{SbCl_3}p_{Cl_2}}{p_{SbCl_5}} = 3.5 \times 10^{-4}
\]

\[
p_{Cl_2} = \frac{(0.20)p_{Cl_2}}{0.15} \]

\( p_{Cl_2} = 2.6 \times 10^{-4} \text{ bar} \)