Chemistry 146 Lecture Problems
Free Energy Calcuations for HBr

Calculate ΔG under the following conditions for the reaction

$H_2 + Br_2$ <--> 2 HBr

$kJ := 10^3 \cdot joule$

$T := 298.15 \cdot K$

$R := 8.314 \cdot joule \cdot K^{-1}$

First calculate ΔG^o for standard pressures

$\Delta G_{f\_HBr} := -53.45 \cdot kJ \cdot mole^{-1}$

$\Delta G_{f\_H2} := 0 \cdot kJ \cdot mole^{-1}$

$\Delta G_{f\_Br2} := 0 \cdot kJ \cdot mole^{-1}$

$\Delta G_{rxn\_std} := 2 \cdot mole \cdot \Delta G_{f\_HBr} - \left(1 \cdot mole \cdot \Delta G_{f\_H2} + 1 \cdot mole \cdot \Delta G_{f\_Br2}\right)$

$\Delta G_{rxn\_std} = -106.9 \cdot kJ$

For this reaction ΔG is negative, so it is spontaneous. This reaction will go forward

Now under the first set of conditions:

$P_{H2} := 1 \cdot atm$

$P_{Br2} := 1 \cdot atm$

$P_{HBr} := 1 \cdot atm$

$$Q := \frac{P_{HBr}^2}{P_{H2} \cdot P_{Br2}}$$

$\Delta G := \Delta G_{rxn\_std} + R \cdot T \cdot \ln(Q)$

$\Delta G = -106.9 \cdot kJ$

Same value as under standard conditions, since all pressures are 1 atm.

The second set of conditions:

$$P_{H2} := 10^{-6} \cdot atm$$

$$P_{Br2} := 10^{-6} \cdot atm$$

$$P_{HBr} := 100 \cdot atm$$

$$Q := \frac{P_{HBr}^{2}}{P_{H2} \cdot P_{Br2}}$$

$$\Delta G := \Delta G_{rxn\_std} + R \cdot T \cdot \ln(Q)$$

$$\Delta G = -15.57693 \cdot kJ$$

The concentration of the reactants is much lower, and the product is much higher, as a result ΔG is less negative. The reaction is still spontaneous in the forward direction, but much closer to equilibrium.

The third set of conditions:

$$P_{H2} := 10^{-8} \cdot atm$$

$$P_{Br2} := 10^{-8} \cdot atm$$

$$P_{HBr} := 500 \cdot atm$$

$$Q := \frac{P_{HBr}^{2}}{P_{H2} \cdot P_{Br2}}$$

$$\Delta G := \Delta G_{rxn\_std} + R \cdot T \cdot \ln(Q)$$

$$\Delta G = 15.23285 \cdot kJ$$

After additional change in the pressure of the product and the reactant, this system now has a positive ΔG. As a result the reaction will proceed spontaneously in the reverse direction.