Solutions to "Kinetics and Equlibrium Problem Set

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Bone Pile:

$kJ := 10^{3} \cdot joule$

$R := 8.314510 \cdot joule \cdot K^{-1} \cdot mole^{-1}$

$M := mole \cdot liter^{-1}$

Given the reaction: R <--> 2 P

Start with the following information:

The forward reaction has

$E_{a\_f} := 2 \cdot kJ \cdot mole^{-1}$

$A_f := 0.01 \cdot s^{-1}$

The reverse reaction has

$E_{a\_r} := 4 \cdot kJ \cdot mole^{-1}$

$A_r := 0.01 \cdot liter \cdot mole^{-1} \cdot s^{-1}$

1.Calculate the rate constant for the forward and reverse reactions at

$T := 298 \cdot K$

From the Arrheius equation:

$$k = A \cdot e^{\frac{-E_a}{R \cdot T}}$$

At $T = 298K$

Forward $\quad k_f := A_f \cdot e^{\frac{-E_{a\_f}}{R \cdot T}} \quad k_f = 4.461 \times 10^{-3}\ s^{-1}$

Reverse $\quad k_r := A_r \cdot e^{\frac{-E_{a\_r}}{R \cdot T}} \quad k_r = 1.99 \times 10^{-3}\ s^{-1}\ mol^{-1}\ liter$

2.Calculate the initial rate of the forward and reverse reaction at these two temperatures given an initial concentration

a. $C_R := 0.1 \cdot M$

$C_P := 0.0 \cdot M$

Forward and reverse rate at $T = 298K$

$Rate_f := k_f \cdot C_R$ $\qquad Rate_f = 4.461 \times 10^{-4} M \cdot s^{-1}$

$Rate_r := k_r \cdot C_P^2$ $\qquad Rate_r = 0 M \cdot s^{-1}$

b. $C_R := 0.0 \cdot M$

$C_P := 0.1 \cdot M$

Forward and reverse rate at $T = 298K$

$Rate_f := k_f \cdot C_R$ $\qquad Rate_f = 0 M \cdot s^{-1}$

$Rate_r := k_r \cdot C_P^2$ $\qquad Rate_r = 1.99 \times 10^{-5} M \cdot s^{-1}$

3.Calculate the rate of the forward and reverse reactions at 298 K and predict the direction of the net reaction when

a

$C_R := 0.1 \cdot M$

$C_P := 0.0 \cdot M$

Forward and reverse rate at $T = 298K$

$Rate_f := k_f \cdot C_R$ $\qquad Rate_f = 4.461 \times 10^{-4} M \cdot s^{-1}$

$Rate_r := k_r \cdot C_P^{\,2}$ $\qquad Rate_r = 0\, M \cdot s^{-1}$

Forward rate constant is faster so the reactioin will go forward.

b.

$C_R := 0.1 \cdot M$

$C_P := 0.1 \cdot M$

Forward and reverse rate at $T = 298K$

$Rate_f := k_f \cdot C_R$ $\qquad Rate_f = 4.461 \times 10^{-4} M \cdot s^{-1}$

$Rate_r := k_r \cdot C_P^{\,2}$ $\qquad Rate_r = 1.99 \times 10^{-5} M \cdot s^{-1}$

Forward rate constant is faster so the reaction will go forward.

c.

$C_R := 0.1 \cdot M$

$C_P := 0.5 \cdot M$

Forward and reverse rate at $T = 298K$

$Rate_f := k_f \cdot C_R$ $\qquad Rate_f = 4.461 \times 10^{-4} M \cdot s^{-1}$

$Rate_r := k_r \cdot C_P^{\,2}$ $\qquad Rate_r = 4.975 \times 10^{-4} M \cdot s^{-1}$

Reverse rate constant is faster so the reaction will go backwards.

d. $C_R := 0.0 \cdot M$

$C_P := 0.1 \cdot M$

Forward and reverse rate at $T = 298K$

$Rate_f := k_f \cdot C_R \qquad Rate_f = 0\,M \cdot s^{-1}$

$Rate_r := k_r \cdot C_P^{\,2} \qquad Rate_r = 1.99 \times 10^{-5} M \cdot s^{-1}$

Reverse rate constant is faster so the reaction will go backwards.

e. $C_R := 0.2 \cdot M$

$C_P := 0.2 \cdot M$

Forward and reverse rate at $T = 298K$

$Rate_f := k_f \cdot C_R \qquad Rate_f = 8.922 \times 10^{-4} M \cdot s^{-1}$

$Rate_r := k_r \cdot C_P^{\,2} \qquad Rate_r = 7.961 \times 10^{-5} M \cdot s^{-1}$

Forward rate constant is faster so the reaction will go forwards.

4.Write an expression for

a.the equlibrium constant for this reaction.

$$K = \frac{(C_B)^2}{C_A}$$

b.the rate of the forward reaction

$$Rate_f = k_f \cdot C_A$$

. c.the rate of the reverse reaction

$$Rate_r = k_r \cdot (C_B)^2$$

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5.At equlibrium, the rate of the forward and reverse reactions are equal. Combine the above expressions as appropriate and solve for the equlibrium constant K.

At equlibrium, the forward and reverse reaction rates are equal.

$$Rate_f = Rate_r$$

Substitute in from the rate expressions

$$k_f \cdot C_A = k_r \cdot (C_B)^2$$

Rearrange to give an expression for concentration of A

$$C_A = k_r \cdot \frac{{C_B}^2}{k_f}$$

The equlibrium expression

$$K = \frac{(C_B)^2}{C_A}$$

Substitute in the expression for the concentration of A found above

$$K = \frac{(C_B)^2}{k_r \cdot \frac{{C_B}^2}{k_f}}$$

Simplify the expression to give the equlibrium constant (K) in terms of the forward and reverse rate constants.

$$K = \frac{1}{k_r} \cdot k_f$$

6.Based upon the value for K at 298 K, calculate the equlibrium concentration of B when [A]=0.1 M. Calculate the rate of the forward and reverse reactions and predict the direction of the net reaction at these concentrations.

$$K := \frac{1}{k_r} \cdot k_f \qquad K = 2.242\ \text{M}$$

$$K = \frac{{C_P}^2}{C_R}$$

$$C_R := 0.1 \cdot \text{M}$$

$$C_P := \sqrt{K \cdot C_R} \qquad C_P = 0.473\ \text{M}$$

$$Rate_f := k_f \cdot C_R \qquad Rate_f = 4.461 \times 10^{-4}\ \text{M} \cdot \text{s}^{-1}$$

$$Rate_r := k_r \cdot {C_P}^2 \qquad Rate_r = 4.461 \times 10^{-4}\ \text{M} \cdot \text{s}^{-1}$$

The rate of the forward and reverse reaction are the same so there is no net reaction.

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