

Kinetics and Reactor Design HW9

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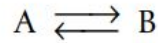
Assigned: April 4, 2023

Due: April 18, 2023

1 Problem Statement

1.1 P11-2_A

P11-2_A For elementary reaction

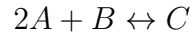


the equilibrium conversion is 0.8 at 127°C and 0.5 at 227°C. What is the heat of reaction?

Figure 1

1.2 Question 2

Derive an expression for the equilibrium constant $K_C(T)$ solely as a function of $K_C(T_1)$, $\Delta \varepsilon \lambda \tau \alpha C_P$, $\Delta H_{Rx}^o(T_R)$, T , T_1 , T_R , and the gas constant R for the following reaction:



2 Problem Solution

2.1 P11-2_A

$$r_A = k(C_A - \frac{C_B}{K_C}) = 0 \quad (1)$$

$$C_A = C_{A0}(1 - X), C_B = C_{A0}X \quad (2)$$

$$r_A = k(C_{A0}(1 - X) - \frac{C_{A0}X}{K_C}) = 0 \text{ at } X = X_e \quad (3)$$

$$(1 - X_e) = \frac{X_e}{K_C} \quad (4)$$

$$K_C = \frac{X_e}{1 - X_e} \quad (5)$$

$$K_C(T_2) = K_C(T_1) \exp \left[\frac{\Delta H_{Rx}^o}{R} \times \left(\frac{1}{T_1} - \frac{1}{T_2} \right) \right] \quad (6)$$

$$\frac{X_{e2}}{1 - X_{e2}} = \frac{X_{e1}}{1 - X_{e1}} \exp \left[\frac{\Delta H_{Rx}^o}{R} \times \left(\frac{1}{T_1} - \frac{1}{T_2} \right) \right] \quad (7)$$

$$\Delta H_{Rx}^o = -23.05 \text{ kJ/mol} \quad (8)$$

2.2 Question 2

$$\Delta H_R(T) = H_{Rx}^o(T_R) + \int_{T_R}^T (C_P)_{prod} dT - \int_{T_R}^T (C_P)_{react} dT \quad (9)$$

$$\Delta H_R(T) = H_{Rx}^o(T_R) + \int_{T_R}^T (C_P)_C dT - \int_{T_R}^T (C_{P_B} + 2C_{P_A}) dT \quad (10)$$

$$\ln \frac{K_C(T)}{K_C(T_1)} = \frac{\Delta H_R(T)}{R} \left(\frac{1}{T_1} - \frac{1}{T} \right) \quad (11)$$

$$= \frac{H_{Rx}^o(T_R) + \int_{T_R}^T (C_P)_C dT - \int_{T_R}^T (C_{P_B} + 2C_{P_A}) dT}{R} \left(\frac{1}{T_1} - \frac{1}{T} \right) \quad (12)$$