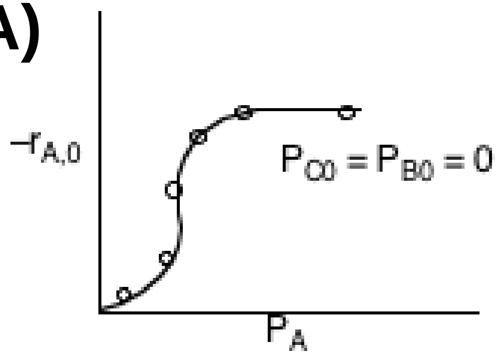
Catalytic Mechanisms

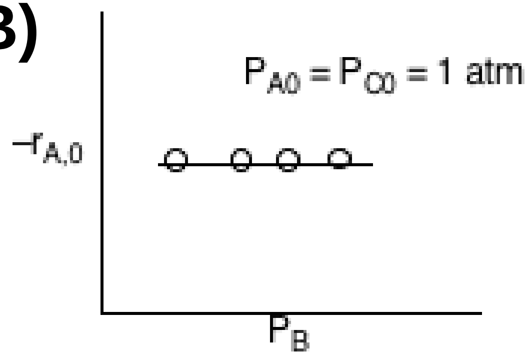
$$2A \underset{\text{cat}}{\rightleftarrows} B + C$$

(a) The initial rate of reaction is shown below

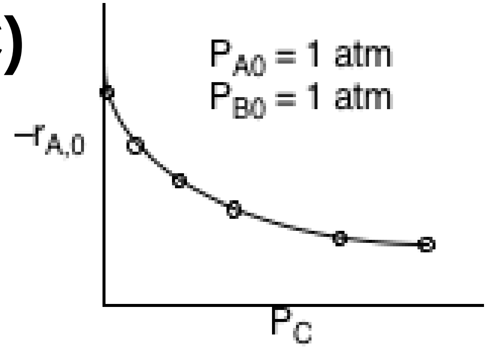
(A)



(B)



(C)



Catalytic Mechanisms

$$A \rightleftarrows B + C$$

(A)

$$-r_A = \frac{kP_A}{1 + K_A P_A + K_B P_B}$$

(B)

$$-r_A = \frac{kP_A}{(1 + K_A P_A + K_C P_C)}$$

(A)

$$A + S \rightleftarrows A \bullet S$$

$$A \bullet S \longrightarrow B \bullet S + C$$

$$B \bullet S \rightleftarrows B + S$$

(B)

$$A + S \rightleftarrows A \bullet S$$

$$A \bullet S \longrightarrow B + C \bullet S$$

$$C \bullet S \rightleftarrows C + S$$

Catalytic Mechanisms

$$2A \rightleftarrows B + C$$

(C)

$$-r_A = \frac{kP_A^2}{\left(1 + K_A P_A + K_C P_C\right)^2}$$

(D)

$$-r_A = \frac{kP_A^2}{\left(1 + K_A P_A + K_C P_C\right)^2}$$

(C)

$$A + S \rightleftarrows A \bullet S$$

$$A \bullet S + A(g) \longrightarrow B + C \bullet S$$

$$C \bullet S \rightleftarrows C + S$$

(D)

$$A + S \rightleftarrows A \bullet S$$

$$A \bullet S + A \bullet S \longrightarrow B + S + C \bullet S$$

$$C \bullet S \rightleftarrows C + S$$

Catalytic Mechanisms

$$2A \longrightarrow B + C$$

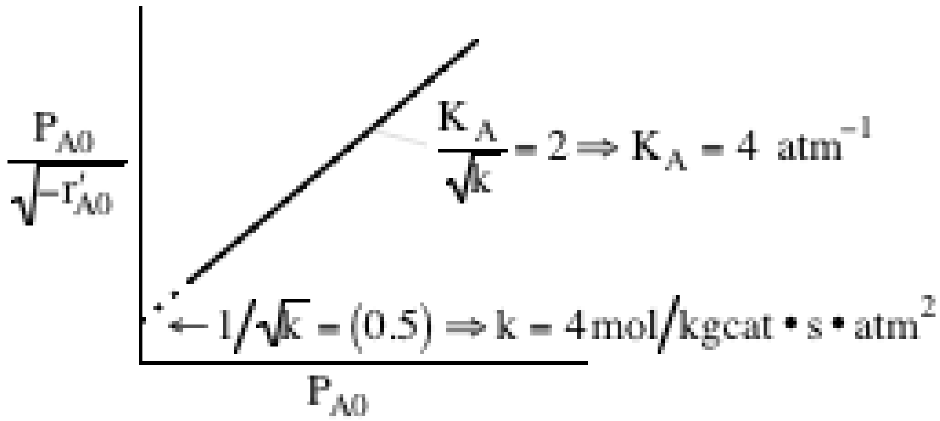
$$A + S \rightleftarrows A \bullet S$$

$$A \bullet S + A \bullet S \longrightarrow B + C \bullet S$$

$$C \bullet S \rightleftarrows C + S$$

$$-r'_A = \frac{kP_A^2}{\left(1 + K_A P_A + K_C P_C\right)^2}$$

Catalytic Mechanisms



$$-r'_{A0} = \frac{4P_A^2}{1 + 4P_{A0} + K_C P_{C0}}$$

For $P_{C0} = 2$ atm and $P_{A0} = 1$ atm, then $-r'_{A0} = 0.0138 \frac{\text{mol}}{\text{kgcat} \bullet \text{s}}$

$$-r'_{A0} = \frac{4}{(1 + 4 + 2K_C)^2} = 0.0138$$

One equation and one unknown

$$K_C = 6\ \text{atm}^{-1}$$

$$-r'_{A0} = \frac{4P_A^2}{(1 + 4P_A + 6P_C)^2}$$

Catalytic Mechanisms

$$2A \rightleftarrows B + C$$

$$A + S \rightleftarrows A \bullet S \qquad -r'_A = r_{A0} = k_A\left[P_A C_V - \frac{C_{A\bullet S}}{K_A}\right] \Rightarrow C_{A\bullet S} = K_A P_A C_V$$

$$A \bullet S + A \bullet S \rightleftarrows B + S + C \bullet S \qquad -r'_A = r_S = k_S C_{A\bullet S}^2$$

$$C \bullet S \rightleftarrows C + S \qquad -r_A = r_{DC} = k_{DC}\left[C_{C\bullet S} - P_C C_V K_C\right] \Rightarrow C_{C\bullet S} = K_C P_C C_V$$

Where K_A = 4 atm^{-1} and K_C = 6 atm^{-1}

1) At what is the ratio of sites with A adsorbed to those sites with C adsorbed when the conversion is 50%?
2) What is the conversion when the sites with A adsorbed are equal to those with C adsorbed?

Catalytic Mechanisms

$$2A \longrightarrow B + C$$

$$A \longrightarrow \frac{B}{2} + \frac{C}{2}$$

$$K_A = 4 \text{ and } K_C = 6$$

Ratio of site concentrations

$$\frac{C_{A\bullet S}}{C_{C\bullet S}} = \frac{K_A\ P_A\ C_V}{K_C\ P_C\ C_V} = \frac{K_A\ P_A}{K_C\ P_C}$$

$$P_A = P_{A0}(1 - X)/(1 + \varepsilon X)$$

$$P_C = P_{A0}\frac{X}{2(1 + \varepsilon X)}$$

$$\frac{C_{A\bullet S}}{C_{C\bullet S}} = \frac{K_A\ P_{A0}\left(\frac{1 - X}{1 + \varepsilon X}\right)\frac{P}{P_0}}{K_C\ P_{A0}\left(\frac{X/2}{1 + \varepsilon X}\right)\frac{P}{P_0}} = 2\frac{K_A(1 - X)}{K_C\ X}$$

Catalytic Mechanisms

1) At X = 0.5

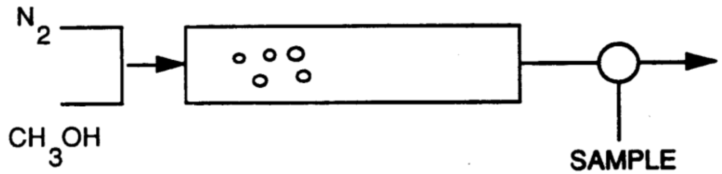
$$\frac{C_{A\bullet S}}{C_{C\bullet S}} =\sim \frac{(2)(4)(1-0.5)}{6(0.5)} = 1.33$$

2) At an equal concentrations of A and C sites, the conversion will be

$$\frac{C_{A\bullet S}}{C_{C\bullet S}} = 1 = \frac{2K_A(1-X)}{K_C\ X}\ , \quad \text{then} \quad X = \frac{2K_A}{K_C + 2K_A} = \frac{(2)(4)}{6+(2)(4)} = \frac{8}{14}$$

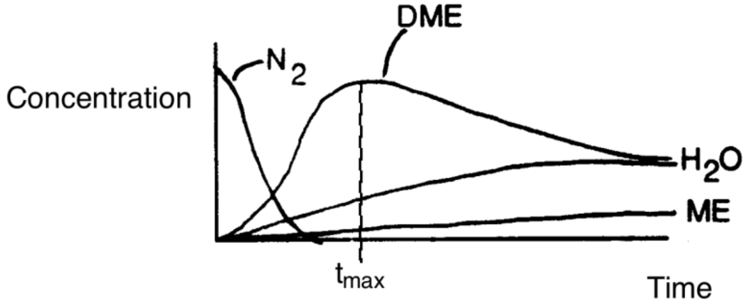
$$X = 0.57$$

Dimethyl Either



$$2CH_3OH \longrightarrow CH_3 - O - CH_3 + H_2O$$

$$2ME \longrightarrow DME + W$$



Initially water does not exit the reactor the same as DME because

Which of the following best describes the data

- **A** There is more DME than water.
- **B** Steady state has been reached.
- **C** Water reacts with ME.
- **D** Water is adsorbed on the surface.