Reaction Mechanisms

Many reactions occur in steps…!
Rate Limiting Step – An Analogy!!

• Consider the Assembly Hall at the U. of I.
• A + 2B \rightarrow AB_2 \quad \text{Rate} = k[A][B]

• A “reaction mechanism” is a series of steps by which the reaction occurs, and the steps can occur at different rates:
  
  • Step 1 \quad A + B \rightarrow AB \quad \text{(Slow)}
  
  • Step 2 \quad AB + B \rightarrow AB_2 \quad \text{(Fast)}
  
  • Overall \quad A + 2B \rightarrow AB_2

• Each step is called an “elementary step”
• AB is an “intermediate” – a substance that is part of the mechanism but doesn’t show up in the balanced equation
\[ A + 2B \rightarrow AB_2 \quad \text{Rate}=k[A][B] \]

- **Step 1**  \[ A + B \rightarrow AB \quad \text{(Slow)} \]
- **Step 2**  \[ AB + B \rightarrow AB_2 \quad \text{(Fast)} \]
- **Overall**  \[ A + 2B \rightarrow AB_2 \]

The rate law for an elementary step can be written from the coefficients in the elementary step:

- For Step 1 the rate law is: \[ \text{Rate}=k[A][B] \]
- For Step 2 the rate law is: \[ \text{Rate}=k[AB][B] \]

**Key Concept** – the slow step is the *rate determining step*

- The rate of the slow step is the rate of the overall reaction
- The rate law of the slow step is consistent with the rate law of the overall reaction
Reaction Mechanisms…Another Example

• **Step 1**  \(2A \rightarrow A_2\)  (SLOOOOOOOOOOOOOW!)
• **Step 2**  \(A_2 + X \rightarrow A_2X\)  (Fast!)
• **Step 3**  \(A_2X + B \rightarrow A_2B + X\)  (Fast!)

• What would the overall reaction be (balanced equation)?
• Overall  \(2A + B \rightarrow A_2B\)
• What would the rate law be??
• Rate = \(k[A]^2\)
• What are \(A_2\) and \(A_2X\)?
• Intermediates!!
• What is \(X\)?
• A Catalyst!!
• Note – intermediates do not appear in the rate law
Reaction Mechanisms…Practice Problem 1

• For the reaction $3X + 2Y \rightarrow X_3Y_2$ the rate law is $\text{Rate} = k[X]^2[Y]$.

• The following mechanism is proposed:

  • Step 1: $X + Y \rightarrow XY$
  • Step 2: $2X + Y \rightarrow X_2Y$
  • Step 3: $XY + X_2Y \rightarrow X_3Y_2$

• Which is the rate limiting step?
• What is (are) the intermediates?
Reaction Mechanisms…Practice Problem 2

- For the reaction $2A + 2B \rightarrow A_2B_2$ the rate law is $\text{Rate}=k[A]^2$

- Two proposed mechanisms are:

  - Mechanism 1:
    - Step 1 $2A + B \rightarrow A_2B$ Slow
    - Step 2 $A_2B + B \rightarrow A_2B_2$ Fast

  - Mechanism 2:
    - Step 1 $2A \rightarrow A_2$ Slow
    - Step 2 $A_2 + B \rightarrow A_2B$ Fast
    - Step 3 $A_2B + B \rightarrow A_2B_2$ Fast

- Which mechanism is consistent with the rate law?