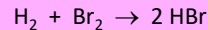


Reaction Mechanism

- A detailed description of the pathway of a chemical reaction
- Not many reactions occur in a single step
- Usually, a series of steps
 - Each step has an activated complex and a unique E_a
 - The slowest step is the **rate determining step**
 - it controls the rate of the overall reaction

Ex: Overall Reaction



Reaction Mechanism



Reaction Rate Law

- Expresses the effect of the concentration of each reactant on the rate
- Determined by experiment only
- [] = molar concentration

Ex: $2\text{H}_2 + 2\text{NO} \rightarrow \text{N}_2 + 2\text{H}_2\text{O}$

At constant volume, temp, [NO]:
doubling $[\text{H}_2]$, doubles rate **and** tripling $[\text{H}_2]$, triples rate

At constant volume, temp, $[\text{H}_2]$:
double [NO], 4x rate **and** triple [NO], 9x rate

For this reaction, the rate law is:

$$\text{Rate} = k[\text{H}_2][\text{NO}]^2$$

k = rate constant

Ex: $\text{A} + \text{B} \rightarrow \text{C}$

	[A] ₀	[B] ₀	Initial rate of formation of C
1	0.20	0.20	2.0×10^{-4} M/min
2	0.20	0.40	8.0×10^{-4}
3	0.40	0.40	1.6×10^{-3}

a) Write the rate law

$$\text{Rate} = k[\text{A}][\text{B}]^2$$

b) Calculate the rate constant

$$2.0 \times 10^{-4} \text{ M/min} = k[0.20][0.20]^2 \quad k = \mathbf{0.025}$$

$$8.0 \times 10^{-4} \text{ M/min} = k[0.20][0.40]^2 \quad k = 0.025$$

$$1.6 \times 10^{-3} \text{ M/min} = k[0.40][0.40]^2 \quad k = 0.025$$

c) If initial concentration of both A and B are 0.30M, what is the rate?

$$\begin{aligned} \text{Rate} &= k[\text{A}][\text{B}]^2 \\ &= 0.025(0.30)(0.30)^2 \\ &= \mathbf{6.8 \times 10^{-4} \text{ M/min}} \end{aligned}$$

Reaction Order of a Reactant

- The exponent on the reactant concentration in the rate law
- Ex: According to the previous rate law:
It is first order in A and second order in B

Overall Reaction Order

- The sum of all the reactant orders
- Ex: The reaction above has an overall reaction order of 3 (that's 1+2)

Ex: Determine the rate law for the reaction $A + B \rightarrow C$, given the following data:

[A] ₀	[B] ₀	[C] After 10 minutes	Rate of production of C
0.100	0.100	0.015	1.5×10^{-3}
0.200	0.100	0.030	3.0×10^{-3}
0.300	0.100	0.045	4.5×10^{-3}
0.100	0.300	0.045	4.5×10^{-3}

Analysis: Rate is directly proportional to [A] and [B] both.

$$\text{Rate} = k[A][B]$$

Ex: Determine the rate law for the reaction $X + Y \rightarrow Z + W$, given the following data:

[X] ₀	[Y] ₀	Rate of production of Z
0.100	0.100	1.5×10^{-3}
0.200	0.100	3.0×10^{-3}
0.100	0.200	6.0×10^{-3}
0.200	0.200	1.2×10^{-2}

Analysis: Rate is directly proportional to [X], but has a squared effect to [Y]

$$\text{Rate} = k[X][Y]^2$$

Ex: $2\text{NO} + \text{O}_2 \rightarrow 2\text{NO}_2$ $\text{Rate} = k[\text{NO}]^2[\text{O}_2]$

At a temperature of 500°C, the rate of production of NO₂ has been found to be 0.010 M/min when the concentration of NO and O₂ are 0.50 M each.

a) What is the value of the specific rate constant at this temp?

$$k = \frac{\text{Rate}}{[\text{NO}]^2[\text{O}_2]} = \frac{0.010\text{M/min}}{(0.050\text{M})^2(0.50\text{M})} = 0.080\text{L}^2/\text{mol}^2\text{min}$$

b) What is the rate of production of NO₂ at 500°C, when the concentration of NO is 0.10M and the concentration of O₂ is 0.30M?

$$\begin{aligned} \text{Rate} &= k[\text{NO}]^2[\text{O}_2] \\ &= (0.080\text{L}^2/\text{mol}^2\text{min})(0.10\text{M})^2(0.30\text{M}) \\ &= 2.4 \times 10^{-4} \text{ mol/Lmin} \\ &= 2.4 \times 10^{-4} \text{ M/min} \end{aligned}$$

Arrhenius Equation

Combines three factors:

- number of particles with E_a or more
- number of collisions per second
- number of collisions with correct orientation

$$k = Ae^{-E_a/RT}$$

constant = 8.314 J/mol K
 Kelvin temp
 activation energy
 frequency factor (#collisions/orientation)
 rate constant