

## Rate Equation [HL]

*Experimentally determined! Not from the balanced equation!*

Rate equation relates rate of reaction to concentration of reactants

rate =  $k[A]^X$  for the reaction  $A \rightarrow B$

The X superscript is **not** the coefficient from the balanced equation.

How to determine experimentally?

- run multiple reactions/experiments varying the concentration of the reactants
  - ~keep at least one concentration constant from one reaction to the next
- determine X from experimental data
  - ~if conc. doubles and rate doesn't change,  $X=0$
  - ~if conc. doubles and rate is x2,  $X=1$
  - ~if conc. doubles and rate is x4,  $X=2$
- solve for k by plugging in experimental data to new equation

Order of Reaction:

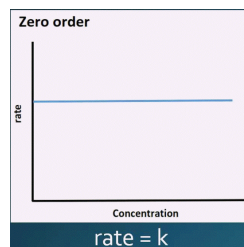
- sum of the superscripts within a rate equation

-ie rate =  $[A]^2[B]^2$  has an order of 4

0th order reactions are not concentration dependent.

-Rate is constant

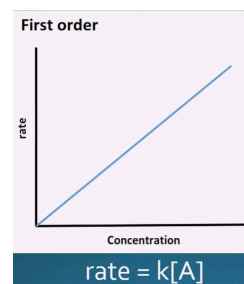
rate =  $k[A]^0$



1st order reactions are concentration dependent

-Rate increases at a constant value as conc. Increases

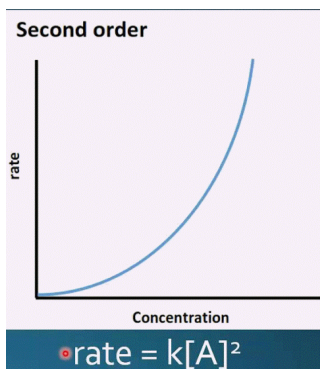
rate =  $k[A]$



2nd order reactions are concentration dependent

-Rate increases at an increasing value as conc. increases (parabolic)

rate =  $k[A]^2$



## Reaction Mechanisms [HL]

### Reaction Mechanism

A set of steps that describe how a reaction occurs at the molecular level; must be consistent with the rate law for the reaction

### Elementary Step

Molecular-level view of a single process taking place in a chemical reaction

### Intermediate

Species produced in one step of a reaction and consumed in a subsequent step

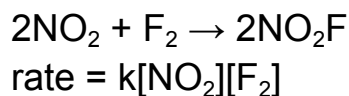
### Rate Determining Step

The slowest step in a reaction mechanism

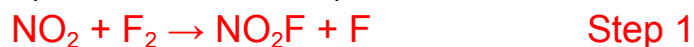
This slow step determines the overall rate

- each step in a mechanism can have a **maximum** of two molecules/atoms interacting
- mechanisms can never be **directly** observed, only deduced from experimental evidence
- one of the steps **must agree** with the rate equation

ex.



This reaction is too complex to occur in one step. We need to break it down into smaller steps:



Compare the steps to the rate equation (determined experimentally)



Step 1 matches the rate equation for the overall equation

-Step 1 is the slow, rate-determining step



→ Catalysts *change* the mechanism of a reaction

~decreases the total  $E_a$  for the reaction, which increases the rate of rxn

## Arrhenius Equation [HL]

-Can be used to calculate the activation energy ( $E_a$ ) for a reaction

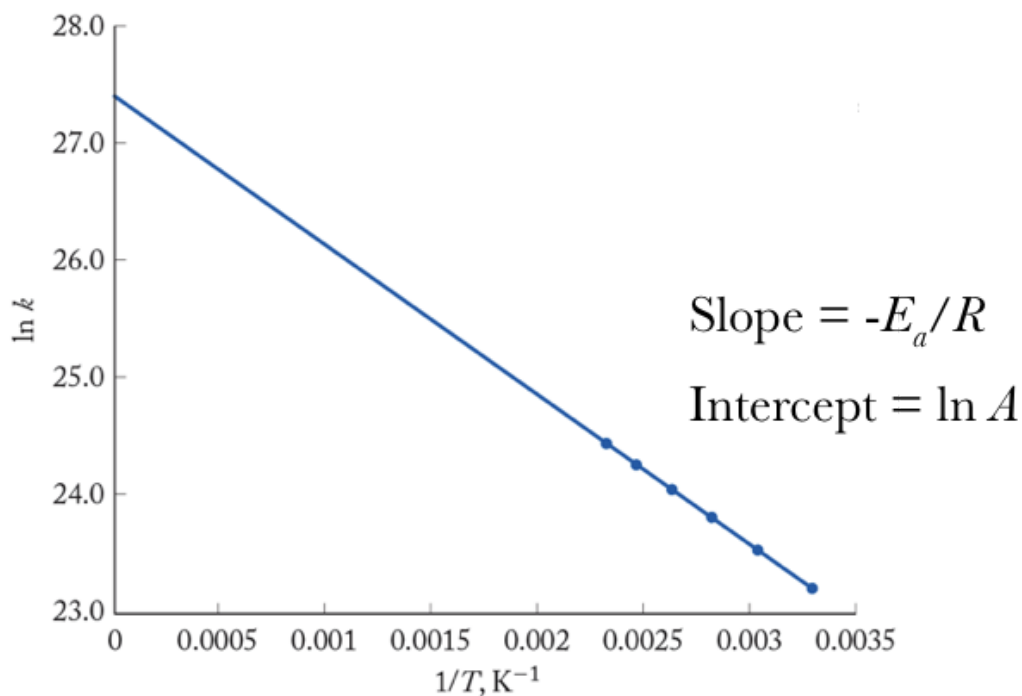
$$k = Ae^{\frac{-E_a}{RT}} \text{ or } k = A \exp\left(\frac{-E_a}{RT}\right)$$

Where A is the 'frequency factor' and R is  $8.31 \text{ J K}^{-1} \text{ mol}^{-1}$

Can be written in a more useful form,

$$\ln(k) = \frac{-E_a}{R} \times (1/T) + \ln A$$

Which can be used to represent this graphically, where  $y = \ln k$ ;  $m = -E_a/R$ ;  $x = 1/T$ ; and  $b = \ln A$



In general, a high activation energy means that the rate is slower.

-Catalysts will increase the value of k within a rate equation