

## Reaction Mechanisms

**Reaction Mechanism:**

**Elementary reactions/steps:**

**Molecularity:**

- The number of molecular species that are involved in a single reaction step
- A theoretical concept which can only be applied to elementary reactions

**Unimolecular:**

**Bimolecular:**

**Termolecular:**

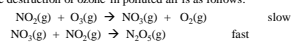
**Rate Determining Step (RDS)**

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**Intermediate**

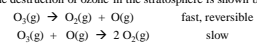
- A short lived molecular species that is \_\_\_\_\_ in one elementary step and \_\_\_\_\_ in a \_\_\_\_\_ elementary step. Does not appear in the net reaction or rate law.

1. A reaction mechanism for the destruction of ozone in polluted air is as follows:



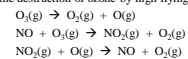
Write a balanced equation for the overall reaction. Define the molecularity of each elementary reaction, and write the rate law for this process. Identify intermediates and catalysts, if any.

2. The reaction mechanism for the destruction of ozone in the stratosphere is shown below.



Write a balanced equation for the overall reaction. Define the molecularity of each elementary reaction, and write the rate law for this process. Identify intermediates and catalysts, if any.

3. The reaction mechanism for the destruction of ozone by high flying aircraft is as follows:



Write a balanced equation for the overall reaction. Define the molecularity of each elementary reaction for this process. Identify intermediates and catalysts, if any.

## Collision Theory

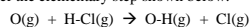
*Product formation can only take place when there are "effective" collision between reactants*

- Not all collisions result in a chemical reaction.
- Collisions that result in a chemical reaction are called "effective collisions"

Two conditions for product formation must be met for molecular collisions to be effective:

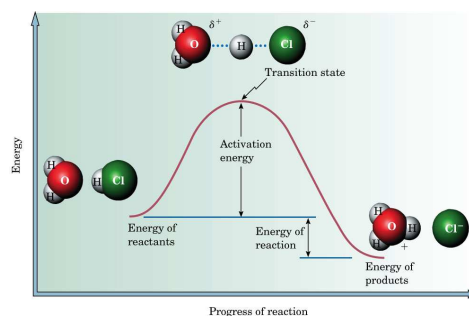
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**Example:** Consider the elementary step shown below.



**Activation Energy ( $E_a$ )** the minimum energy necessary for a specific reaction to occur

**Energy Level Diagram** shows the reaction progress vs. Potential Energy (P.E)  
Indicates the relative energy of the following:  
i) reactants, ii) transition state (TS), and iii) products

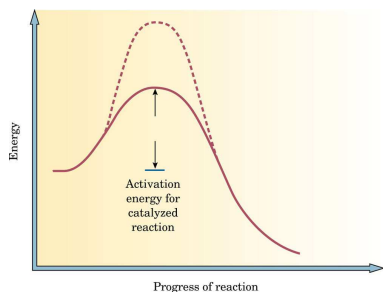


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## Catalyst

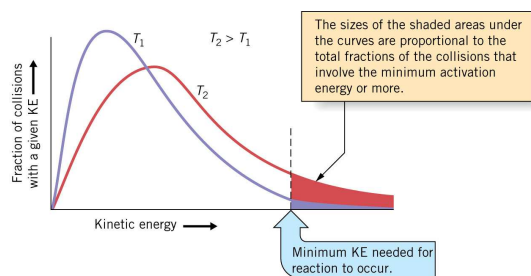
A substance that is added to increase the rate of a chemical reaction without being used up during the reaction

- A catalyst is \_\_\_\_\_ in one elementary step, and \_\_\_\_\_ in the same form in a \_\_\_\_\_ step.
- Speeds up the chemical reaction by providing an \_\_\_\_\_ for the reaction that lowers the \_\_\_\_\_ → more collision have enough energy to overcome the \_\_\_\_\_ → reaction rate increases



## Temperature

As temperature increases, Kinetic Energy increases, leading to higher reaction rates



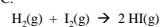
## The Arrhenius Equation

Temperature is included in the rate law via the rate constant, k. Arrhenius discovered that the temperature dependence of the rate constant, could be described by an exponential equation.

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

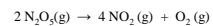
- Write the straight line form of the Arrhenius Equation.
- How could the activation energy and pre-exponential factor be graphically obtained?
- Derive the equation that relates the activation to k at two different temperatures.

- The rate constants for formation of HI were measured at the two different temperatures shown below. Calculate the activation energy, pre-exponential factor, and specific rate constant for formation of HI at 427 °C.



k	temperature
$2.7 \times 10^{-4}$	327°C
$3.5 \times 10^{-3}$	377°C
?	427°C

- The rate constants for the decomposition of gaseous dinitrogen pentoxide are  $3.7 \times 10^{-5} \text{ s}^{-1}$  at 25 °C and  $1.7 \times 10^{-3} \text{ s}^{-1}$  at 55 °C.



- What is the activation energy for this reaction in kJ/mol? ( $1.0 \times 10^5 \text{ kJ/mol}$ )
- What is the rate constant at 35 °C? ( $1.4 \times 10^{-4} \text{ s}^{-1}$ )
- What is the numerical value of the pre-exponential factor, A? ( $5.3 \times 10^4 \text{ s}^{-1}$ )