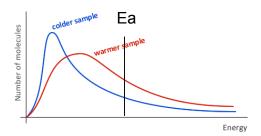
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### TRANSITION STATE THEORY

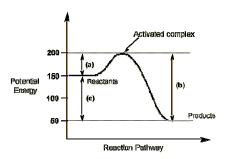
- looks at transition between reactants to products.
- i.e. K.E. is converted to potential energy as the reactants collide

#### **POTENTIAL ENERGY DIAGRAM**

diagrammatic way of representing P.E. as a reaction progresses

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**Exothermic**: reactants have higher energy level than products



The activation energy (E<sub>a</sub>) for the forward reaction is shown by (a):

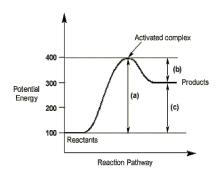
The activation energy  $(E_a)$  for the reverse reaction is shown by **(b)**:

The enthalpy change for the reaction is shown by **(c)**:

•

- •
- •
- •

Endothermic: reactants energy is lower than products



The activation energy (E<sub>a</sub>) for the forward reaction is shown by (a):

The activation energy (E<sub>a</sub>) for the reverse reaction is shown by **(b)**:

The enthalpy change for the reaction is shown by **(c)**:

- top of Ea:
- · activated complex -
- Occurs during the **transition state** of the reaction

## **CATALYSIS DEMONSTRATION**

In this demonstration the reaction between rochelle salt (sodium potassium tartrate,  $KNaC_4H_4O_6 \cdot 4H_2O$ ) and hydrogen peroxide produces carbon dioxide. The reaction can be qualitatively followed, by observing the rate of production of bubbles of gas. The reaction is catalysed by  $Co^{2+}$ , which forms a reaction intermediate.

## Questions and Observations

| 1.  | Why was the solution of rochelle salt and hydrogen peroxide heated?            |
|---|--|
| 2.  | Why was the solution divided?  |
| 3.  | After the solution was divided, what evidence was there for a chemical change? |
| 4.  | Describe the CoCl <sub>2</sub> solution catalyst.                              |
| 5.  | Should the catalyst be added to the reaction solution or vice versa?           |
| 6.  | What did you observe after the catalyst was added?                             |
| _   |  |
| 7.  | In your own words, define the term catalyst.                                   |
| 8. Predict what will happen when the contents of the beaker are added to the "control" beaker |  |

## 6.4 REACTION MECHANISMS AND CATALYSTS

most chemical reactions proceed over a number of steps

#### **ELEMENTARY REACTIONS**

**Reaction Mechanism** 

.

#### **Elementary reaction**

:

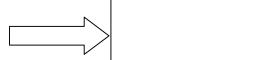
• ie. can involve formation of different molecules or ions or a change in energy or geometry of starting molecules.

e.g. 
$$2NO_{(g)} + O_{2(g)}$$
  $\rightarrow$   $2NO_{2(g)}$ 

2 steps involved

(1) 
$$NO_{(g)} + O_{2(g)} \longrightarrow NO_{3(g)}$$

(2) 
$$NO_{3(g)} + NO_{(g)}$$
  $\longrightarrow$   $2NO_{2(g)}$ 



o Presence of intermediate would help explain the mechanism

## **Molecularity of Elementary Reactions**

Molecularity ⇒

e.g. previous had 2 molecules colliding at each step

∴ bimolecular -

unimolecular - 1 particle reacts (Cl<sub>2</sub> light 2Cl)

termolecular -

(rare to have it happen)

#### RATE LAW EQUATIONS FOR ELEMENTARY REACTIONS

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eg. A product Rate = 
$$K[A]$$
2A product Rate =  $K[A]^2$ 

- · Reaction mechanisms -
- •

Look for a possible colour change if intermediate is present, and has that colour.

In order for a mechanism to be proposed it must fulfill the following criteria:

- 1.
- 2.
- 3.

## **RATE DETERMINING STEP**

ie. assembly line analogy - only as fast as the slowest guy

How does the rate determining step relate to rate law of overall?

Eg. 
$$2NO_{2(g)} + Cl_{\overline{2(g)}}$$
  $\triangleright$   $2NO_2Cl_{(g)}$   
Rate = k[NO<sub>2</sub>][Cl<sub>2</sub>]

Proposed mechanism:

1.

2.

reasonable

•

Does the mechanism support the experimentally determined rate law?

: rate of overall reaction depends on rate of slow step

Step 1 Rate<sub>1</sub> =  $k_1[NO_2][Cl_2]$ 

•

eg.  $2NO_{(g)} + 2H_{2\overline{(g)}} \longrightarrow N_{2(g)} + 2H_2O_{(g)}$ 

Rate law is Rate =  $k[NO]^2[H_2]$ 

## Proposed mechanism

Step 1 
$$2NO_{(g)} + H_{2(g)} \longrightarrow N_2O_{(g)} + H_2O_{(g)}$$
 slow

Step 2 
$$N_2O_{(g)} + H_{2(g)} \longrightarrow N_{2(g)} + H_2O_{(g)}$$
 fast

is the proposed mechanism reasonable?

- (A)
- (B)

Step 2 is bimolecular Step 1 is the molecular (rare by possible)

-

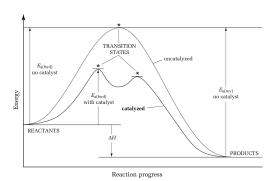
*:*.

•

∴seems reasonable

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# **CATALYSTS** -



How a Catalyst works:

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e.g. A + B AB one step bimolecular reaction

OVERALL 
$$A + B = AB$$

Catalyst - produced in step 1 —> consumed in step 2

Homogeneous Catalysts -

Heterogeneous Catalysts -