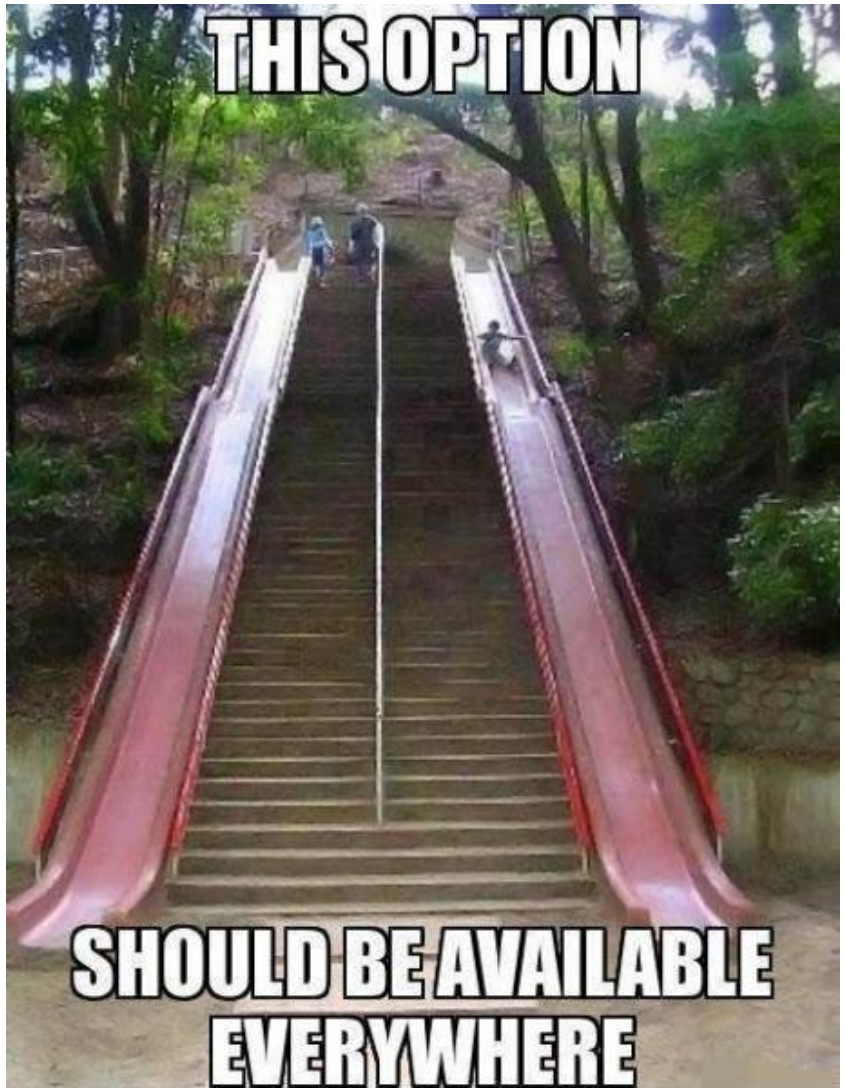
Reaction Mechanisms



Outcomes:

- Explain the concept of a reaction mechanism.

Reaction Mechanisms:

Recall:

In order for a chemical reaction to occur, the reacting particles (molecules/atoms) must **COLLIDE** with each other. If the particles do not **COLLIDE**, **NO** reaction occurs.

Consider the reaction:

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

According to **COLLISION THEORY**, for this reaction to occur in **ONE STEP**, **THREE** particles must collide:

→ ***2 NO molecules and 1 O_2 molecule***

THREE particle **COLLISIONS** are quite **RARE**! Think of making a 2 ball **COMBINATION** shot in **POOL** → much more **DIFFICULT**!

Reaction Mechanisms:

Many things in life occur in a series of **STEPS**:

→ ***Arranging a date***
→ ***Building a car, house, etc.***
→ ***Starting a car, etc.***

Chemical reactions are no different!

Simple Reactions:

- Reactions that occur in just **ONE STEP**.

Complex Reactions:

- Reactions that take place in **MORE** than **ONE STEP**.
- The reaction $2NO_{(g)} + O_{2(g)} \rightarrow 2NO_{2(g)}$ takes **2 STEPS**:

Step 1: $2NO \rightarrow N_2O_2$

Step 2: $N_2O_2 + O_2 \rightarrow 2NO_2$

$N_2O_2 + O_2 + 2NO \rightarrow 2NO_2 + N_2O_2$

The **STEPS** in which a reaction occurs is the **REACTION MECHANISM**.

Reaction Mechanisms:

Compounds like **N_2O_2** (above) that are **PRODUCED**, then **CONSUMED** are called **REACTION INTERMEDIATES.**

The **SUM** of the steps in a **REACTION MECHANISM** will equal the **NET REACTION.**

CATALYSTS are **CONSUMED** at the **START**, then **PRODUCED** at the **END** → are **NOT** in **OVERALL** reaction.

Example:

For the reaction, ***$NO_2 + CO \rightarrow NO + CO_2$***, the mechanism is:

used made

Step 1: ***$NO_2 + \cancel{NO_2} \rightarrow \cancel{NO_3} + NO$ (slow)***

Step 2: ***$\cancel{NO_3} + CO \rightarrow \cancel{NO_2} + CO_2$ (fast)***

used made

Net Reaction: ***$NO_2 + CO \rightarrow NO + CO_2$***

NO_2 = catalyst

NO_3 = intermediate

Reaction Mechanisms:

Rate Determining Step:

- Any process involving steps is only as **FAST** as its **SLOWEST PART**.
- Not all **STEPS** in a **MECHANISM** have the same **RATE**.
- The **SLOWEST** rate is called the **RATE DETERMINING STEP *(RDS)***, and it determines the **OVERALL REACTION RATE**.
- In the above example, **CO** molecules must wait for **INTERMEDIATE** **NO_3** molecules to be **PRODUCED**, before the reaction can **PROCEED**.
- Since the **RDS** affects the **RATE** of the **ENTIRE REACTION** the **MOST**, changes to the **REACTANTS** in the other **STEPS** will have very **LITTLE EFFECT** on the **RATE** of the reaction.

Reaction Mechanisms:

P_2

Example:

Given the following mechanism:

↓

P + Q → ~~X~~ + T	***(slow)***
~~X~~ + P → ~~Y~~ + R	***(fast)***
~~Y~~ + S → T	***(moderate)***

a) What is the net reaction?

$2P + Q + S \rightarrow 2T + R$

b) What are the reaction intermediates?

X, Y

c) Which is the rate determining step?

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d) What would be the effect of increasing the concentration of P?

Rate ↑ (P in RDS)

e) What would be the effect of decreasing the concentration of Q?

Rate ↓ (Q in RDS)

f) What would be the effect of increasing the concentration of S?

No change (not in RDS)