CONCEPT: REACTION MECHANISM

Reaction Mechanism Overview

- A **Reaction Mechanism** is a step-by-step sequence of *elementary steps* by which an overall _____ change occurs.
  - □ **Elementary Step:** ___ step in a series of reactions that show the progress of a reaction at the molecular level.

Reaction Mechanism Overview

_____ Step 1 : $Cl\ (g) + O_3\ (g) \longrightarrow ClO\ (g) + O_2\ (g)$

_____ Step 2 : $ClO\ (g) + ClO\ (g) \longrightarrow Cl\ (g) + ClO_2\ (g)$

Overall Reaction : $ClO\ (g) + O_3\ (g) \longrightarrow ClO_2\ (g) + O_2\ (g)$

_____

- □ **Catalyst:** Compound shown as a _____ in the 1st step and then as a _____ in the final step.
- □ **Reaction Intermediate:** Compound that first appears as a _____ then later as a _____.

EXAMPLE: Consider the following reaction mechanism for the formation of nitrobenzene:

$HNO_3\ (aq) + H_2SO_4\ (aq) \longrightarrow H_2NO_3^+\ (aq) + HSO_4^-\ (aq)$

$H_2NO_3^+\ (aq) + C_6H_6\ (aq) \longrightarrow C_6H_6NO_2^+\ (aq) + H_2O\ (l)$

$C_6H_6NO_2^+\ (aq) + HSO_4^-\ (aq) \longrightarrow H_2SO_4\ (aq) + C_6H_5NO_2\ (aq)$

Identify the reaction intermediate(s) and catalyst(s).

Molecularity

- Associated with the number of moles for _____ molecules within an elementary step.

$1\ CO_2\ (g) + 1\ H_2O\ (l) \longrightarrow 1\ H_2CO_3\ (aq)$

□ **1 mole** = _____molecular □ **2 moles** = _____molecular □ **3 moles** = _____molecular

EXAMPLE: The elementary reaction, $2\ NO_2\ (g) + F_2\ (g) \longrightarrow 2\ NO_2F\ (g)$, is an example of a _____ reaction.

a) Unimolecular b) Trimolecular c) Bimolecular d) Termolecular e) Tetramolecular

CONCEPT: REACTION MECHANISM

Rate Law Determination

● In a reaction mechanism, one of the elementary steps is classified as a *slow step*.

□ **Slow Step:** The _____-determining step that limits the overall rate of a chemical reaction.

- For a slow step, the _____ of the reactants are equal to the reaction orders of the rate law.

EXAMPLE: Consider the following elementary steps. What is the rate law of the reaction mechanism?

$N_2O_5\,(g) \rightleftharpoons NO_3\,(g) + NO_2\,(g)$ [Fast]

$NO_2\,(g) + N_2O_5\,(g) \longrightarrow 3\,NO_2\,(g) + O_2\,(g)$ [Slow]

$NO_3\,(g) + O_2\,(g) \longrightarrow NO\,(g) + O_3\,(g)$ [Fast]

STEP 1: Locate the _____ step of the reaction mechanism.

□ As long as the reactants are not _____, their _____ = the reaction orders of the rate law.

Rate = ___ [ ]□ [ ]□

STEP 2: If a reactant is an _____ cancel it out with the product intermediate.

STEP 3: If Step 2 happens, use the elementary step possessing the product intermediate.

□ For that elementary step the _____ of the reactants still equal the reaction order.

□ For that elementary step the _____ of the products = the _____ of the reaction orders.

Rate = ___ [ ]□ [ ]□

CONCEPT: REACTION MECHANISM

PRACTICE: Consider the following elementary steps:

$NO_2\,(g) + NO_2\,(g) \longrightarrow NO_4\,(g) + NO\,(g)$ [SLOW]

$NO\,(g) + CO_3\,(g) \longrightarrow N\,(g) + CO_4\,(g)$ [FAST]

What is the rate law of the reaction mechanism?

PRACTICE: The following reaction of $2\,Br_2\,(g) + 2\,NO\,(g) \longrightarrow N_2\,(g) + 2\,Br_2O\,(g)$ has the following rate law: Rate = $k\,[Br_2][NO]^2$. The proposed mechanism for the reaction is:

$Br_2\,(g) + NO_2\,(g) \longrightarrow N\,(g) + Br_2O\,(g)$ [SLOW]

$N\,(g) + NO\,(g) \longrightarrow N_2\,(g) + O\,(g)$ [FAST]

$O\,(g) + Br_2\,(g) \longrightarrow Br_2O\,(g)$ [FAST]

Which of the following statements is/are **false**?

a) The rate determining step is bimolecular.

b) There are three elementary steps in the reaction mechanism.

c) The mechanism possesses a catalyst.

d) O is the only reaction intermediate in this reaction mechanism.

e) This is not a valid mechanism for the reaction.