During Class Invention #

Reaction Mechanisms

Name(s) with Lab section in Group

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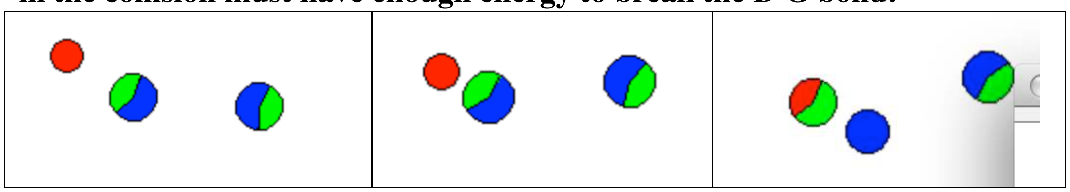
1. Given the chemical equation

$$R + BG \rightarrow RG + B$$

For the reaction to occur above an R atom must collide with a BG molecule. The collision must have the correct orientation, and the particles in the collision must have enough energy to break the B-G bond.



2. Write the general differential form of the rate law for the reaction in Q1 above.

$$\textbf{Rate} = \mathbf{k[R]^1\,[BG]^1}$$

3. Define the terms *reaction mechanism* and *rate determining step*.

A reaction mechanism attempts to describe the stepwise sequence of elementary reactions that take reactants to products. The mechanism describes in detail the bonds that are broken and formed as the reaction proceeds.

Every mechanism consists of a series of stepwise reactions. Each reaction in the mechanism has a rate associated with it. The overall speed of the reaction depends upon the slowest step of the mechanism. The rate law of this step is identical to the experimental rate law. The slow step of the mechanism is also called the rate determining step of the mechanism. The sum of all the steps of the mechanism must equal the overall balanced chemical equation.

4. List several characteristics of a reasonable mechanism for a chemical reaction.

Each elementary step of a mechanism typically involves one, two or three reactants combining to form products. The steps of a mechanism must add together to yield the overall balanced chemical equation. The coefficients of the reactants in the rate determining step of the mechanism must correspond to the exponents, or order of

the reactants in the experimental rate law.

5. Look at the simulation (http://introchem.chem.okstate.edu/DCICLA/K2GBM.htm) for the reaction,

$$2G + B \rightarrow G_2B$$

The rate law is known to be,

$$\text{Rate} = k[G]^2$$

Suggest a possible mechanism for the reaction.

1) $\mathbf{G + G \rightarrow G_2}$
2) $\mathbf{G_2 + B \rightarrow G_2B}$

6. The rate law for following reaction

$$2NO_{2}(g) + F_{2}(g) \rightarrow 2NO_{2}F(g)$$

was experimentally determined to be

$$\text{rate} = k[NO_2]^1[F_2]^1$$

which of the following mechanisms is the most reasonable? Explain your reasoning for making the choice you did.

a) $2NO_{2}(g) + F_{2}(g) \rightarrow 2NO_{2}F(g)$

The experimental rate law indicates the slow step of the mechanism involves the collision of a single NO_2 molecule and a single F_2 molecule. This mechanism has two molecules of NO_2 molecule colliding with a single F_2 molecule. This is not in agreement with the experimental rate equation.

b) $NO_{2}(g) + F_{2}(g) \rightarrow NO_{2}F(g) + F(g)$ (fast)
$NO_{2}(g) + F(g) \rightarrow NO_{2}F(g)$ (slow)

The slow step of this mechanism involves the collision between a fluorine atom and an NO_2 molecule. The rate law for this step would be

$$\mathbf{rate = k[NO_2]^1[F]^1}$$

This does not agree with the experimental rate law.

c) $NO_{2}(g) + F_{2}(g) \rightarrow NO_{2}F(g) + F(g)$ (slow)
$NO_{2}(g) + F(g) \rightarrow NO_{2}F(g)$ (fast)

The rate law for the slow step of this mechanism is;

$$\mathbf{rate = k[NO_2]^1[F_2]^1}$$

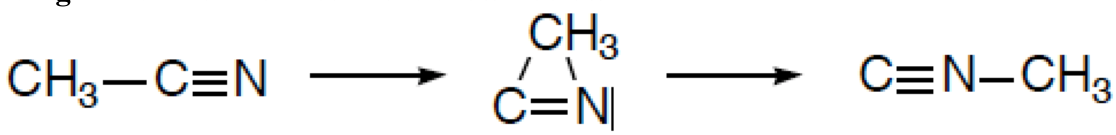
which agrees with the experimental rate law.

7. Suggest a mechanism for the reaction

$$CH_3NC_{(g)} \rightarrow CH_3CN_{(g)}$$

if the experimental rate law is rate = $k[CH_3NC]^1$.

This reaction is a rearrangement of the CH_3, methyl, group. In the reactants, the methyl group is bonded to the carbon atom and, in the product, the methyl group is bonded to the nitrogen atom. Since the reaction is first order, the mechanism consists of a single step. The methyl group must move from the carbon atom to the nitrogen atom through an intermediate where the methyl group interacts with both atoms.
A diagram of the intermediate is shown below.

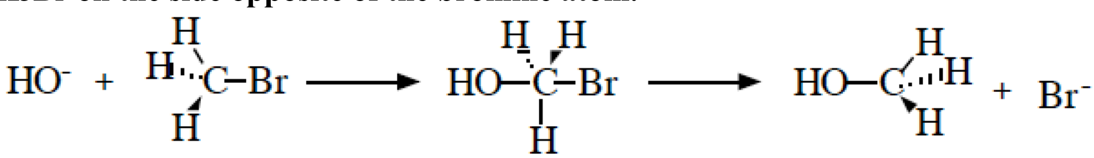


8. Suggest a mechanism for the reaction

$$OH^- + CH_3Br \rightarrow CH_3OH + Br^-$$

if the experimental rate law is rate = $k[CH_3Br]^1[OH^-]^1$.

The mechanism for this reaction is single step. When a hydroxide ion collides with a CH_3Br molecule in the correct orientation, the hydroxide ion displaces the bromide ion forming methanol and bromide ion. The hydroxide ion must collide with the CH_3Br on the side opposite of the bromine atom.



9. Suggest a mechanism for the reaction

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

if the experimental rate law is rate = $k[NO_2]^2$.

In this example, the experimental rate law suggests the slow step of the mechanism involves the collision of two NO_2 molecules. A possible mechanism is shown below,

1) $NO_2(g) + NO_2(g) \rightarrow NO(g) + NO_3(g)$ slow

2) $NO_3(g) + CO(g) \rightarrow NO_2(g) + CO_2(g)$ fast

The elementary steps of the mechanism sum to yield the overall balanced chemical equation. Notice that NO_3 is an intermediate in this mechanism.

10. Consider the following set of equations

Step I: $Cl_{(g)} + O_{3(g)} \rightarrow ClO_{(g)} + O_{2(g)}$

Step II: $ClO_{(g)} \rightarrow Cl_{(g)} + O_{(g)}$

$$O_{3(g)} \rightarrow O_{(g)} + O_{2(g)}$$

Describe the process illustrated by the above set of equations and the role each of the species plays in the process. Use words like mechanism, elementary steps, overall reaction, reactants, products, intermediate, and catalyst in your description.

The mechanism for the decomposition of ozone, O_3, is catalyzed by the presence of chlorine radicals, Cl. The first step in the decomposition is the reaction between $Cl_{(g)}$ and $O_{3(g)}$ to form an intermediate, ClO, and oxygen, O_2. The intermediate decomposes to reform the chlorine radical and an oxygen atom.