Reaction Mechanisms

1. What is a reaction mechanism?

   A reaction mechanism is a series of steps involved in a chemical reaction.

2. A reaction mechanism is comprised of a series of elementary steps. These steps are termed as unimolecular (involving one molecule, bimolecular (involving two molecules) and termolecular (involving three molecules) - which are first order, second order and third order, respectively.

3. Reaction mechanisms must

   a. Add up to yield overall balanced equation.

   b. Agree with experimentally determined rate law.

4. What is the rate determining step?

   The step that determines the rate law is slowest step in the mechanism – a reaction can only move as fast as its slowest component.

5. Write the rate law for the following elementary step

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

   Rate = $k[O_3][O]$

6. What is the rate law and overall balanced equation for the following mechanism?

   $NO_{2(g)} + NO_{2(g)} \rightarrow NO_{3(g)} + NO$ Slow

   $NO_{3(g)} + CO_{(g)} \rightarrow NO_{2(g)} + CO_{2(g)}$ Fast

$$\text{Rate} = k[NO_2][NO_2] = k[NO_2]^2$$

7. What is an intermediate?

An intermediate is a species that is both created and completely used up during the reaction.

8. When do we use the steady state approximation?

The steady state approximation is used when the rate determining step, and therefore rate law, contains an intermediate and the relative speeds of the elementary steps are not known. Because the intermediate does not feature in the balanced reaction equation, it cannot be included in the differential rate law.

9. Find the rate law for the following

$$2NO \leftrightarrows N_2O_2$$
$$N_2O_2 + H_2 \rightarrow N_2O + H_2O$$

$$\text{Rate} = \frac{k_1 k_2 [NO]^2 [H_2]}{(k_{-1} + k_2[H_2])}$$

10. How would the method used and results differed if we had known the relative speeds of reaction for the two elementary steps?

$2NO \rightleftharpoons N_2O_2$ Fast Equilibrium

$N_2O_2 + H_2 \rightarrow N_2O + H_2O$ Slow

$$\text{Rate} = k[NO]^2[H_2]$$