Rate of Reaction and the Collision Theory

Chapter 6.4

Theoretical Models for Chemical Kinetics

- Kinetic-Molecular theory can be used to calculate the collision frequency.
  - In gases 10^{30} collisions per second.
  - If each collision produced a reaction, the rate would be about 10^{6} M s^{-1}.
  - Actual rates are on the order of 10^{4} M s^{-1}.
    - Still a very rapid rate.
  - Only a fraction of collisions yield a reaction.

Activation Energy

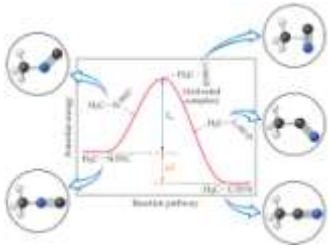
- For a reaction to occur there must be a redistribution of energy sufficient to break certain bonds in the reacting molecule(s).
- Activation Energy is:
  - The minimum energy above the average kinetic energy that molecules must bring to their collisions for a chemical reaction to occur.

Activation Energy

- In other words, there is a minimum amount of energy required for reaction: the activation energy, E_a.
- Just as a ball cannot get over a hill if it does not roll up the hill with enough energy, a reaction cannot occur unless the molecules possess sufficient energy to get over the activation energy barrier.

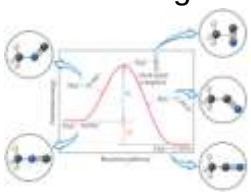
Reaction Coordinate Diagrams

It is helpful to visualize energy changes throughout a process on a reaction coordinate diagram like this one for the rearrangement of methyl isonitrile.



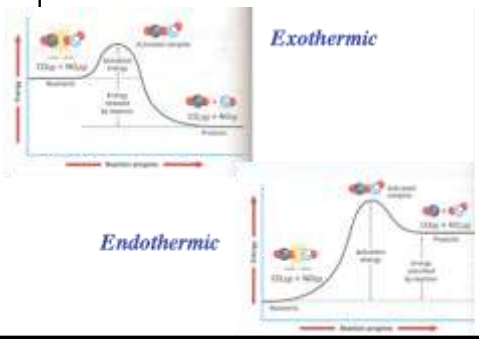
Reaction Coordinate Diagrams

- It shows the energy of the reactants and products (and, therefore, ΔE).
- The high point on the diagram is the transition state.



- The species present at the transition state is called the activated complex.
- The energy gap between the reactants and the activated complex is the activation energy barrier.

Activation Energy Curves



Collision Theory

- If activation barrier is high, only a few molecules have sufficient kinetic energy and the reaction is slower.
- As temperature increases, reaction rate increases.
- Orientation of molecules may be important.

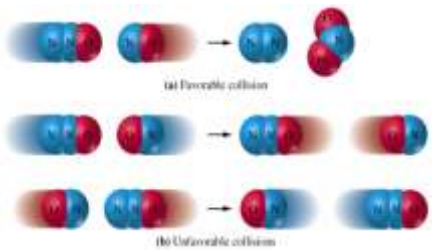
The Collision Model

- In a chemical reaction, bonds are broken and new bonds are formed.
- Molecules can only react if they collide with each other if there is sufficient energy and if the atoms are oriented properly

The Collision Model

Furthermore, molecules must collide with the correct orientation and with enough energy to cause bond breakage and formation.

The Collision Model



The Collision Model

- Collision theory explains why some naturally occurring reactions are immeasurably slow at room temp.
  - Carbon and Oxygen react when charcoal burns, but this reaction has a high activation energy
  - At room temp, the collisions of oxygen and carbon molecules aren't energetic enough to react
  - But the reaction can be helped along a number of ways