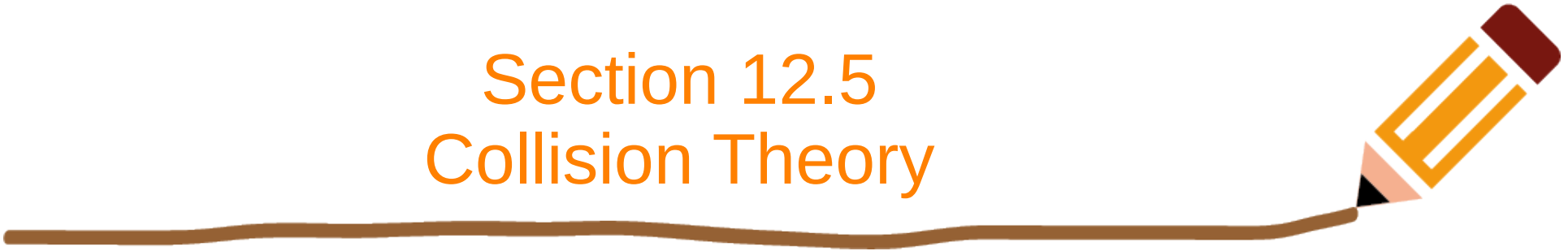
Section 12.5
Collision Theory



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Learning Objectives

- Use the postulates of collision theory to explain the effects of physical state, temperature, and concentration on reaction rates
- Define the concepts of activation energy and transition state
- Use the Arrhenius equation in calculations relating rate constants to temperature

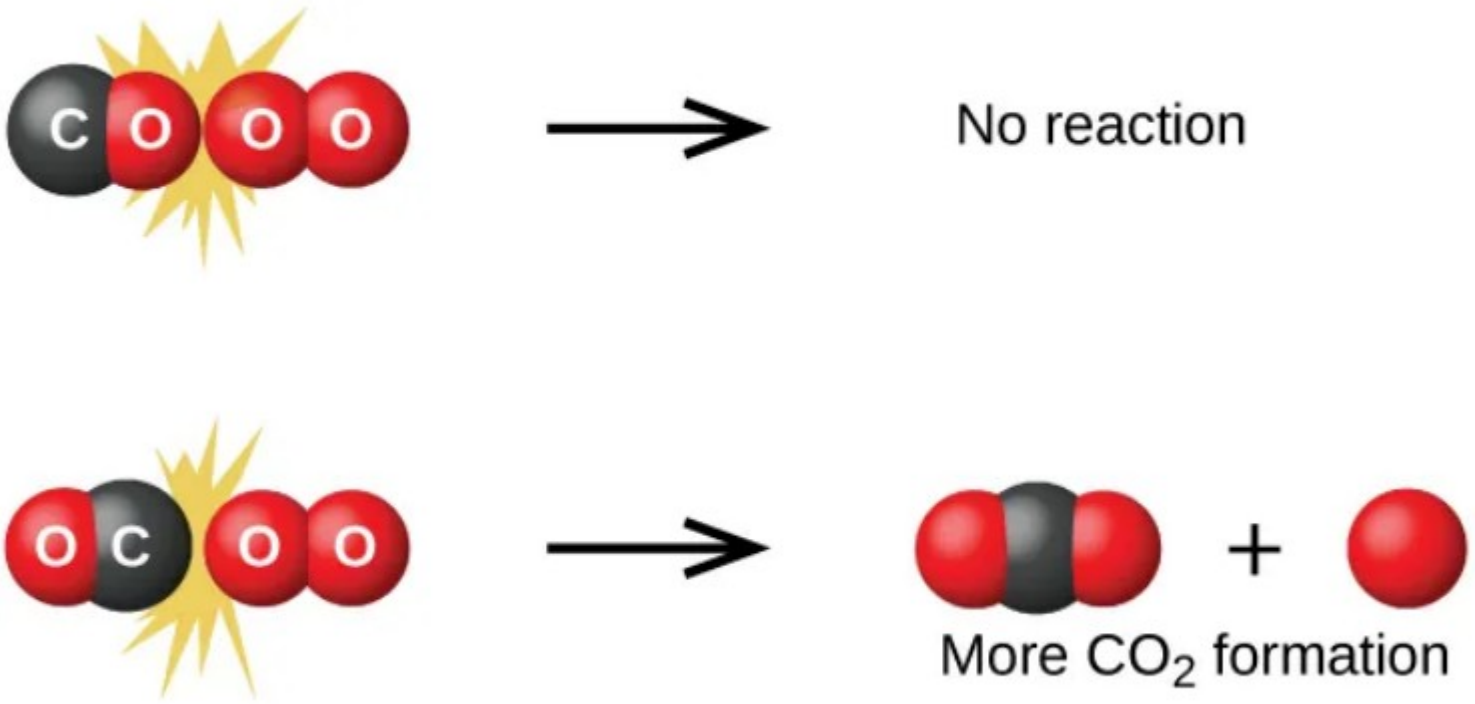
Collision Theory

- Collision Theory is based on the following postulates:
  1) The rate of a reaction is proportional to the rate of reactant collisions:

$$\text{reaction rate} \propto \frac{\#\ \text{collisions}}{\text{time}}$$

  2) The reacting species must collide in an orientation that allows contact between the atoms that will become bonded together in the product.
  3) The collision must occur with adequate energy to permit mutual penetration of the reacting species' valence shells so that the electrons can rearrange and form new bonds.

Orientation Matters



Transition States

- In addition to a proper orientation, the collision must also occur with sufficient energy.
- When reactant species collide with both proper orientation and adequate energy, they combine to form an unstable species called an **activated complex** or a **transition state**.
- These unstable intermediates are difficult to detect but strong evidence has been gathered to confirm their existence.

Collisions and Concentration

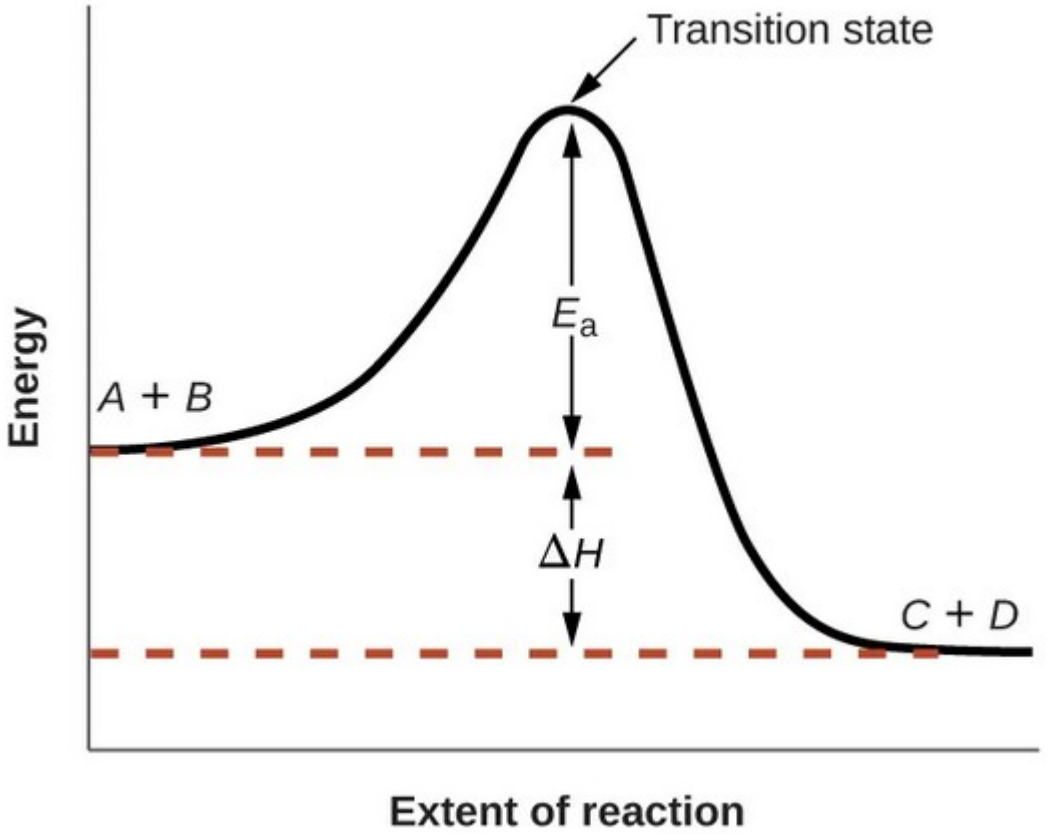
- Most reaction rates increase as concentrations increase.
- Increasing the concentration increases the density of molecules.
- With more molecules packed tighter together the probability of a collision increases.
- This assumes that the molecules have adequate kinetic energy (temperature) to react.

Activation Energy

- The minimum energy necessary to form a product during a collision between reactants is called the **activation energy (Ea).**
- If the average kinetic energy of the molecules is larger than the activation energy, the reaction will proceed quickly.
- If the average kinetic energy is lower than the activation energy, the reaction will proceed slowly.

Reaction Diagrams

- **Reaction Diagrams** are used to visualize the energetics of a reaction.



The Arrhenius Equation

- The **Arrhenius equation** relates the activation energy and the rate constant, *k*, for many chemical reactions:

$$k = Ae^{-E_a/RT}$$

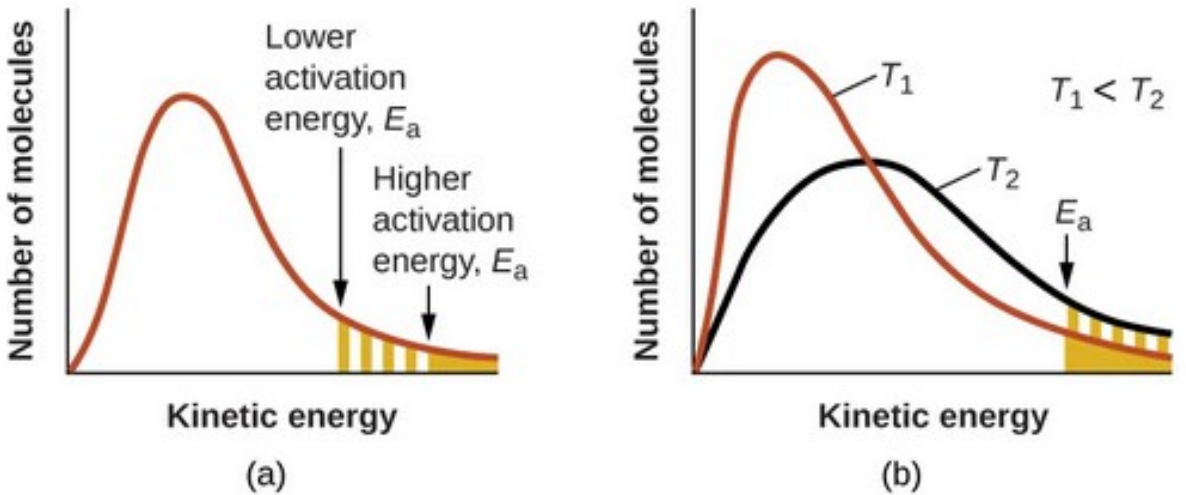
  - *R* is the ideal gas constant, 8.314 $\frac{\text{J}}{\text{mol} \cdot \text{K}}$
  - T is temperature in Kelvin
  - E_a is the activation energy in joules per mole
  - *e* is the constant 2.7183
  - A is a constant called the **frequency factor**

Frequency Factor

- The frequency factor is related to the frequency of collisions and the orientation of the reacting molecules.
- It reflects how well the reaction conditions favor properly oriented collisions between reactant molecules.
- An increased probability of effectively oriented collisions results in larger values for A and faster reaction rates.

Temperature and Activation Energy

- The exponential term of the Arrenhius Equation describes the effect of temperature on reaction rate.
- Higher temperature means a greater fraction of molecules possess sufficient energy (RT) to overcome the activation barrier (E_a).



Linearizing the Arrenhius Equation

- Arrhenius equation can be rewritten to have a linear form:

$$\ln k = \left(\frac{-E_a}{R}\right)\left(\frac{1}{T}\right) + \ln A$$

$$y = mx + b$$

- A plot of ln(*k*) versus 1/T is linear with a slope equal to $-E_a/R$ and a *y*-intercept equal to ln(A).