3.0 Beginning of a Reaction

Molecules that collide frequently with enough energy will form a new molecule, products, assuming they collide in the right orientation.

3.1 Energy Diagrams

Transition state (TS): point in which bond forming and bond breaking occur simultaneously; shown as local maxima on graph.

- Rate of reaction corresponds to the energy from the reactant to the TS known as the energy of activation, E_a

3.3 two-step reaction mechanism

- # of steps = # of transition states

Intermediate: structure that is neither a product nor reactant, but exists definitively for a discrete/limited amount of time.

- # of intermediates = # of TSs - 1

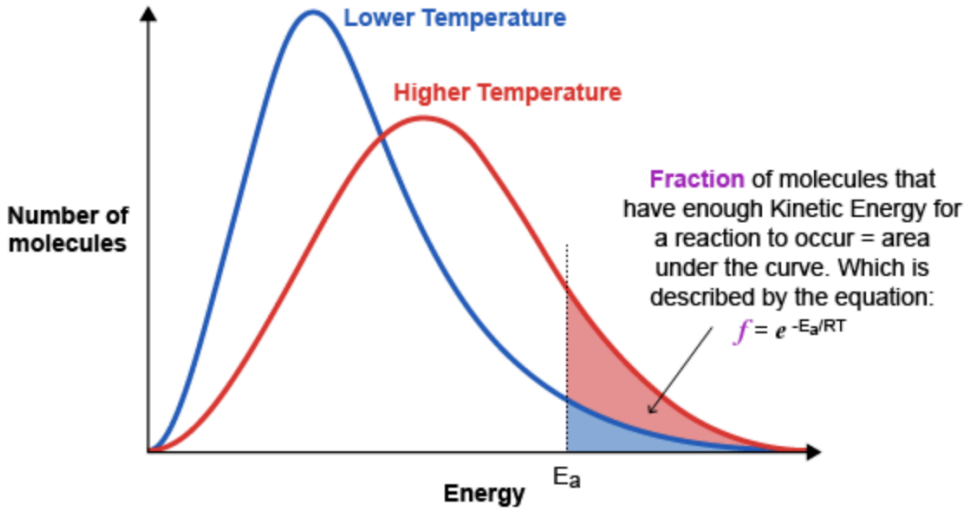
3.4 Energy of Activation

Energy of activation (E_a): the energy barrier that reactants must overcome to form products; it is measured as the difference between energy of transition state and energy of reactants. **The reaction's E_a is the TS with the greatest magnitude of energy,** and is thus known as the **rate-limiting step.**

- A greater E_a corresponds to a slower rate (inversely proportional)

Other factors affecting the reaction rate:

- Concentration: the **greater the concentration** of reactants in the rate-limiting step, **the faster** the reaction rate. Greater concentrations come with a greater chance for collision.
- Temperature: **The higher the temp, the greater the rate.** Temp corresponds to kinetic energy thus greater temp is greater kinetic energy required to surmount E_a.



At higher temperatures, more molecules have enough energy to surpass the E_a. **That's all you need to know about this graph.**

3.5 Catalysts

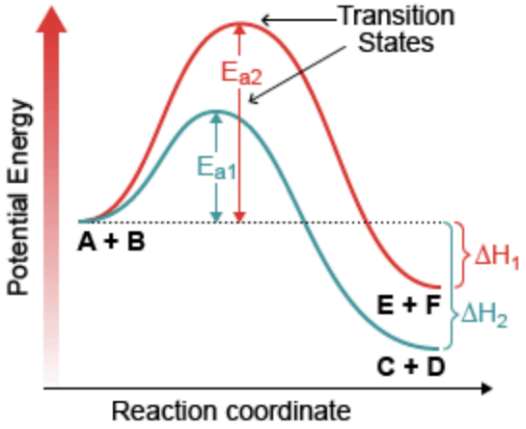


Figure 3.12. Energy diagram showing two possible pathways for the reaction between A and B. [12]

Catalyst: substance that increases the rate of the reaction by changing its pathway (adding more steps). **It reduces E_a, but does not affect H or G.**

- Catalyst is not changed

3.6 Hammond Postulate - Transition State appearance

Hammond postulate: TS resembles the closest stable species (product, reactant, intermediate).

3.7 kinetics vs thermodynamics

Kinetics: rate of reaction

- Kinetic control - the pathway with the lower E_a (faster)

Thermodynamics: relative energy between products and reactants.

- Thermodynamic control - the pathway with the greater ΔH

The kinetically favorable pathway can also be the thermodynamically favorable pathway; they're not mutually exclusive!

3.8 Rate Laws

Rate law is a measure of how much an individual reactant affects the rate of the reaction.

$$\text{Rate} \propto [A]^x[B]^y$$

$$\text{Rate} = k[A]^x[B]^y$$

Equation 3.1

- The k is a rate constant that is specific to each reaction, always positive.

- The exponents are reaction orders for each individual reactant. The overall reaction order is a sum of each individual reaction order.