

Collision Theory

Temperature

- Increasing the temperature increases the rate of all reactions.
- Temperature relates to the motion of particles.
- If you speed them up they are more likely to bump into each other.
- The current model state that reactants must collide with each other to react and form products.

Collision Theory

- Collision Theory- explains why reactions occur.
- Reactions are the result of energetic collisions of atoms/molecules.
- Collisions must be energetic enough and at the proper orientation to break the stable electron configuration of the reactants.

Collision Theory

- Reaction rates are the result of frequent and energetic molecular collisions.
- The more moles (higher concentration) of reactants present, the increased likelihood of a collision.
- Rate depends on the number of collisions.

But not all collisions...

- Increasing the temperature increases the average speed of the reactants.
- This in turn increases the frequency of the collisions.
- Although, calculations and experiments lead us to believe only a fraction of collisions result in a reaction.

Starting...

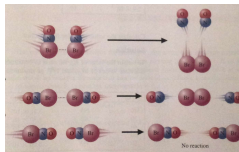
- Why doesn't a book of matches burst into flames?
- Particles are moving. Collisions are happening.
- This is an **exothermic** reaction. Much like a nuclear chain reaction, the heat from one reaction is the energy needed for many more to start.
- If you have reaction that starts another and continue at an exponential rate...

Activation Energy

- Atoms are held together by chemical bonds.
- Some bonds are stronger than others.
- The bond strength is determined by the amount of energy required to break it.
- The collisions of molecules provide energy.
- Weaker collisions don't have enough energy to break bonds.
- Activation Energy-** the minimum amount of energy needed to break bonds to begin a reaction

Probability ...Randomness

- Collisions above the activation energy alone do not guarantee a reaction.
- The collisions still must be at
 - a proper orientation
 - to cause a reaction.



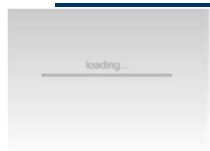
Equilibrium

- Higher Temperature always results in more collisions.
- For an exothermic reaction, E_a (fwd) is always greater than E_a (rev).
- Exothermic reactions take **high energy reactants** and make **low energy products**.
- The energy is the bond energy.

Molecular structure

- Collisions are labeled as *effective* or *ineffective*.
- Effective collision increase the rate as particles line up in such a way that a reaction occurs upon collision.
- Ineffective collisions do not start a reaction at all.
- That is why reactive chemicals can sit next to each without a danger.
- E.g. match, dynamite

The Gas Phase Reaction of NO and Cl₂



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Transition State Theory

- describes the role of energy in reaction rates.
- Moving particles have mostly KE with little PE.
- When particles collide KE decreases and PE increases as Intermolecular Attractions (IMA) increase.
- If the PE meets or exceeds E_a , then a reaction occurs as bonds are broken and made.

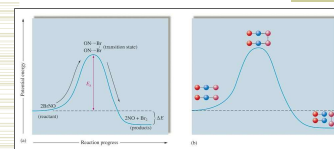
Transition State

- Transition State Theory claims that species form that are neither a product nor reactant, but something in between.
- This unstable, momentary species is called the activated complex or transition state.
- Therefore, E_a is used to stretch and deform bonds in order to reach a transition state.

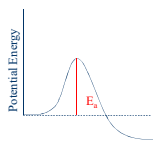
Transition States and Activation Energy

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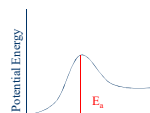
Change in Potential Energy



Exothermic Reaction



Endothermic Reaction



Effect of temperature on reaction rate

- Arrhenius was able to express k , rate law constant as a function of the temperature.
- He also had to factor in a value A , which is the frequency factor.
- Frequency factor is the rate of successful collisions

Arrhenius Equation

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

A = frequency factor
 E_a = activation energy
 R = gas constant (8.3145 J/K·mol)
 T = temperature (in K)

AP Learning Objective

The Arrhenius equation can be used to summarize experiments on the temperature dependence of the rate of an elementary reaction and to interpret this dependence in terms of the activation energy needed to reach the transition state.

XX Calculations involving the Arrhenius equation are *beyond the scope* of this course and the AP Exam.

Linear Form of Arrhenius Equation

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

- This form helps because it is now in the form of $y = mx + b$
- The slope is $-E_a/R$, the y intercept is $\ln(A)$

Change in temperature

- We can further manipulate this if we look for a change in temperature, ΔT or $T_2 - T_1$
- $\ln(k_2/k_1) = E_a(1/T_1 - 1/T_2) / R$
- In this manipulation, we canceled out A

Activation Energy

- The gas-phase reaction between methane and diatomic sulfur is given by the equation
- $\text{CH}_4(\text{g}) + 2\text{S}_2(\text{g}) \rightarrow \text{CS}_2(\text{g}) + 2\text{H}_2\text{S}(\text{g})$
- At 550°C the rate constant for this reaction is 1.1 L/mol s , and at 625°C the rate constant is 6.4 L/mol s . Using these values, calculate E_a for this reaction.

Catalysts

- a substance that increases the reaction rate without being consumed in the reaction.
- A catalyst speeds up the forward and reverse reactions. A reaction with a catalyst **DOES NOT YIELD MORE PRODUCT**, but rather achieves the end point at a faster **RATE**.

- A catalyst **LOWERS THE ACTIVATION ENERGY** by providing a **different mechanism** that requires less energy.
- However, in this mechanism the catalyst will be cancelled out.
- Normally, the rate determining step has a high energy bond that is difficult to break.

Catalyst example

- $2\text{O}_3 \rightarrow 3\text{O}_2$
- Ozone will decompose into elemental oxygen.
- Here is a mechanism without a catalyst
- $\text{O}_3 \rightarrow \text{O} + \text{O}_2$ slow
- $\text{O} + \text{O}_3 \rightarrow 2\text{O}_2$ fast
- The first step is slow. There is no collision to start the reaction

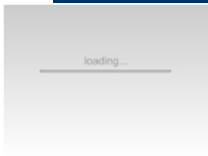
Catalyst example

- $2\text{O}_3 \rightarrow 3\text{O}_2$
- Here is a mechanism with a catalyst
- $\text{O}_3 + \text{Cl} \rightarrow \text{ClO} + \text{O}_2$
- $\text{ClO} + \text{O}_3 \rightarrow \text{Cl} + 2\text{O}_2$
- ClO is an intermediate
- Chlorine is a catalyst because it is a reactant in the first step, but a product in the last step. So it isn't used up during the reaction.
- Chlorine changed the mechanism, altering the slow step.

Heterogeneous/Homogeneous Catalysis

- This is only talking about the phase the substances in the reaction.
- Homogeneous catalysis has the reactants and catalyst in the same phase. Liquid and a liquid.
- Heterogeneous catalysis has the reactants and catalyst in a different phase. Gas and a solid.

Homogeneous Catalysis



loading...

Inhibitor

- Is the reverse of a catalyst.
- Inhibitors increase the activation energy of a reaction by blocking the mechanism for a reaction.