Chemistry 6A F2007

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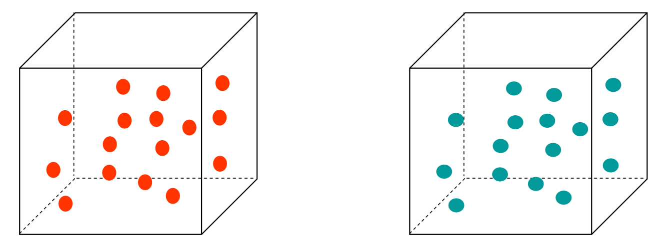
Chemical Kinetics measure the *rate* of appearance of products or the rate of disappearance of reactants.

Reactants $\rightarrow$ Products

Reactants go away with time…. Products appear with time….



The rate of appearance or disappearance is measured in units of *concentration* vs. *time*.

$$\text{Rate} = \frac{\text{moles}/\text{L}}{\text{time}} = M\cdot s^{-1} \text{ or } M\cdot min^{-1}$$

etc…

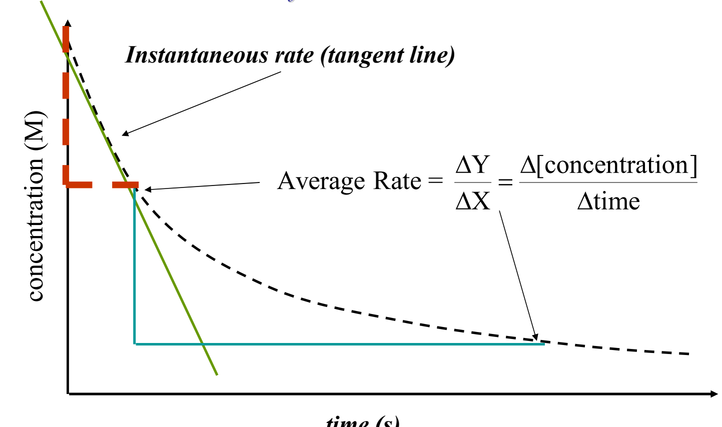
There are three "types" of rates

1. *initial rate*
2. *average rate*
3. *instantaneous rate*

Reaction Rates

During the begining stages of the reaction, the initial rate is very close to the instantaneous rate of reaction.

Initial rate



Reaction Rates:

Reaction Rate: The change in the concentration of a reactant or a product with time ($M{\cdot}s^{-1}$).

$$\text{Reactant} \rightarrow \text{Products}$$
$$A \rightarrow B$$

$$\text{Average rate} = \frac{\text{change in number of moles of B}}{\text{change in time}}$$

$$= \frac{M\ B_{final} - M\ B_{initial}}{\Delta t} = \frac{\Delta[B]}{\Delta t}$$

Since reactants go away with time: $\text{Rate} = -\frac{\Delta[A]}{\Delta t}$

A reaction generates hydrogen gas (H_2) as a product. The reactants are mixed in a sealed 250 mL vessel. After 15.0 minutes, 3.91×10^{-2} mol H_2 have been generated. Calculate the average rate of the reaction in Ms^{-1}.

The initial concentration of H_2 is zero
After 15.0 min there are 3.91×10^{-2} mols of H_2

C_o = initial concentration

$$\Delta C = C_t - C_o$$

C_t = concentration at some time "t"

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$$\Delta C = C_t - C_o$$

$$\Delta C\ (\text{moles/L}) = \frac{3.91\times10^{-2}\ \text{mols} - 0}{250.0\ \text{mL} \times \frac{10^3\ \text{mL}}{1\text{L}}} = 0.156\ M$$

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$$\text{Rate} = \frac{\Delta[H_2]}{\Delta t} = \frac{\Delta C}{t_f - t_{in}}$$

$$\text{Rate} = \frac{0.156\ M}{(15.0\ \text{min} - 0\ \text{min}) \times \frac{60\ \text{s}}{1\text{min}}} = 1.73\times10^{-4}\ Ms^{-1}$$

Reaction Rate

- A reaction rate measures the speed of a reaction. (How fast)
- Reaction rates must be determined experimentally.
- The rate of reaction must be a function of *concentration*:

•As concentration increases, so do the number of *collisions*…

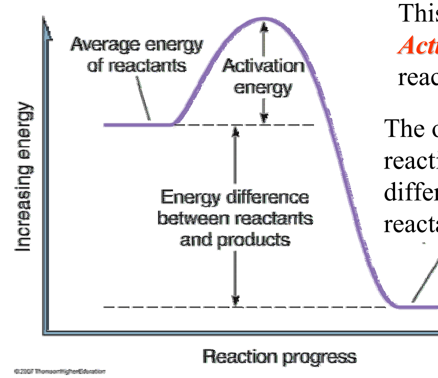
•As the number of collisions increase, so does the *probability* of a reaction.

•This in turn increases the *rate* of conversion of reactants to products. (In most cases)

•In many reactions the collision must have a *"minimum energy"* to activate the reaction.

ACTIVATION ENERGY

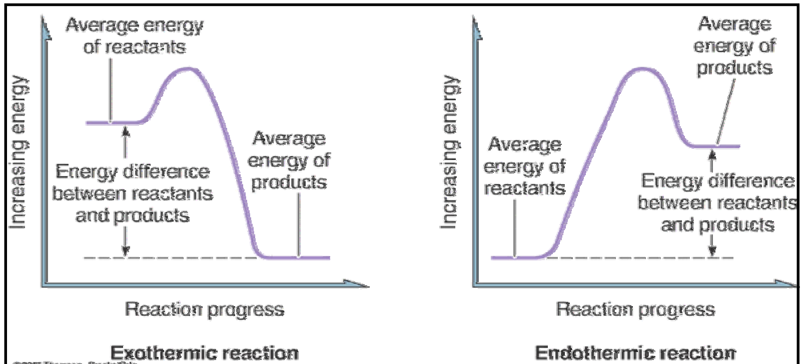
When a reaction is non-spontaneous, the reaction may proceed if it is "kick-started" with a little energy.



This hill is know as the ***Activation Energy*** for the reaction,

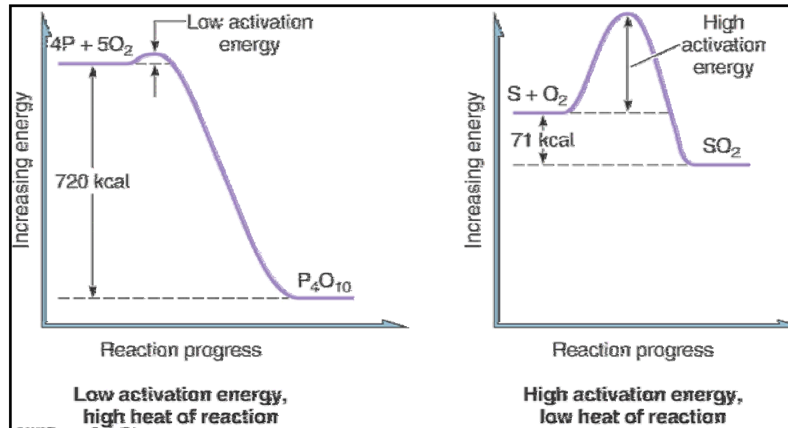
The overall energy of the reaction is determined by the difference between the reactants and products.

In this case, the reaction is ***exothermic***.



In an ***Exothermic*** reaction, the products lie lower in energy than the reactants.

In an ***Endothermic*** reaction, the reactants lie lower in energy than the products.

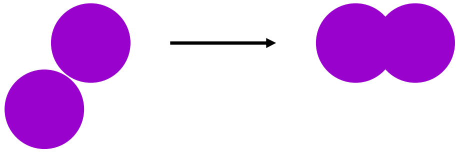


The activation energy of a reaction is unique to the reaction.

Temperature Dependence of a Reaction:

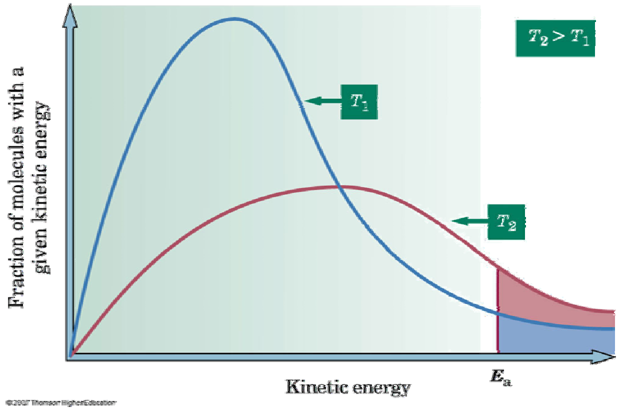
Reactions usually occur at a faster rate when the temperature is increased. ***Why?***

In order for a reaction to occur, the molecules must collide.



If the temperature in increased, then the number of collisions increases!

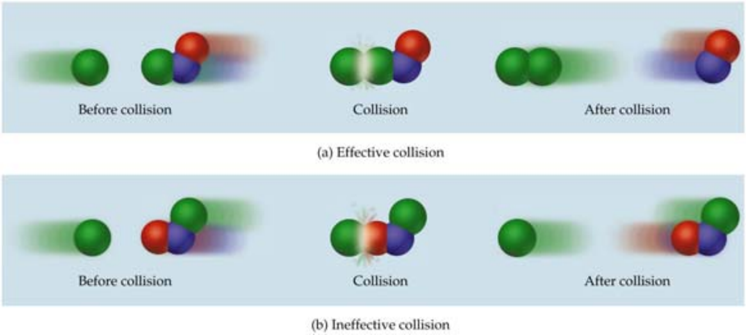
This in turn increases the rate at which the molecules react!



As temperature increases, so does the average velocity (*Kinetic Energy*) of the molecules.
This means there are more molecules that possess the minimum energy (*Activation Energy*) to react.

Orientation factors into the equation

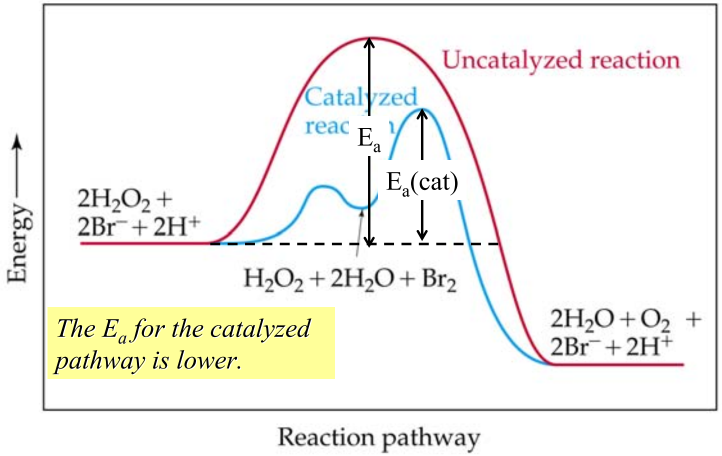
The orientation of a molecule during collision can have a profound effect on whether or not a reaction occurs.



Some collisions do not lead to reaction even if there is sufficient energy.

THE PRESENCE OF CATALYSTS

- *Catalysts* are substances that speed up chemical reactions *without being consumed* in the reaction.
- A ***homogeneous catalyst*** exists in the same phase of the a reaction mixture.
- A ***heterogeneous catalyst*** involves usually, the catalyst as a solid the reaction takes place on the catalyst surface.
- Heterogeneous catalysts generally speed up a reaction by providing an *alternate reaction pathway* with a *lower activation energy* than the normal pathway.
- Solid catalysts provide a surface on which reactant molecules *adsorb* with increasing the rate by reducing orientation requirements.
- Adsorbed molecules with *favorable orientations* are can more easily find one another, this increasing the rate.



The reaction takes a “shortcut”, therefore the rate increases!

A ***heterogeneous catalyst*** exists in a different phase from the reactants.
In the gas phase, $H_2(g) + C_2H_4(g) \rightarrow C_2H_6(g)$ is slow…