Chapter 12.1 - Explaining Chemical Changes

Some reactions do not proceed spontaneously at room temperature unless additional energy is added to start them off.   Why is this initiating energy source necessary to cause the reaction?

From your experience, you may also have noticed that different reactants appear to react at different rates.
For example, different metals in contact with the same acid react at varying rates, and the same metal in contact with different acids reacts at varying rates.
http://chemconnections.org/Java/molecules/index.html (particles- temp, conc, etc.)

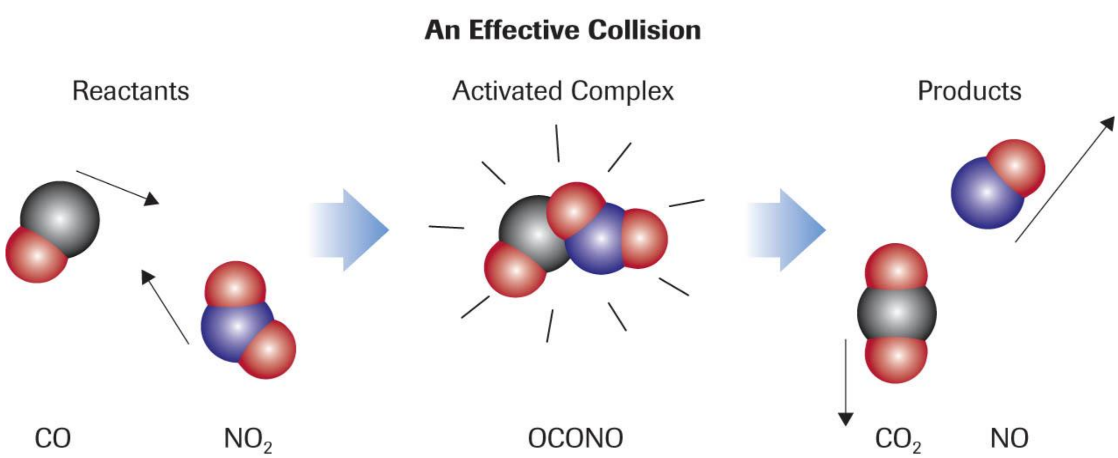
A. Collision-reaction Theory

http://www.mhhe.com/physsci/chemistry/essentialchemistry/flash/collis11.swf (orientation)
http://www.chm.davidson.edu/vce/KineticMolecularTheory/BasicConcepts.html (rxn particle collisions)

Chemists created the collision–reaction theory to describe, explain, and predict characteristics of chemical reactions. Some of the main ideas of the collision–reaction theory are the following: (p525)

- A chemical sample consists of entities that are in constant random motion at various speeds, rebounding elastically from collisions with each other. (Kinetic energy is conserved during elastic collisions.)
- A chemical reaction must involve collisions of reactant entities.
- An effective collision requires sufficient energy. Collisions with the required minimum energy have the potential to react.
- An effective collision also requires the correct orientation (positioning) of the colliding entities so that bonds can be broken and new bonds formed.
- Ineffective collisions involve entities that rebound elastically from the collision.

According to collision–reaction theory, reactions can only take place when entities collide, but not all collisions result in a reaction. If the orientation is correct and the energy is sufficient, then a reaction can occur.



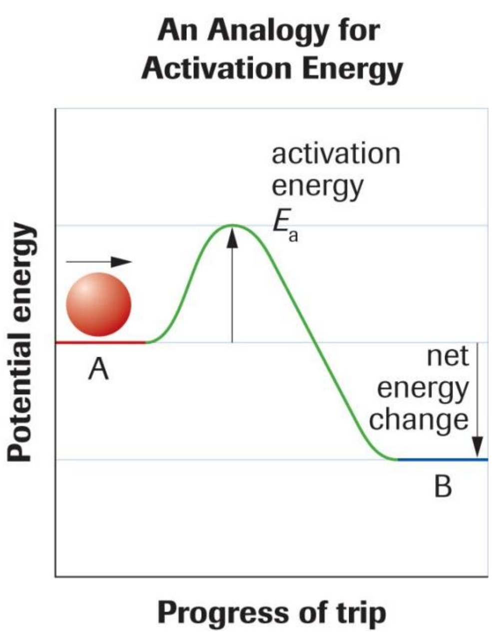
There are two sources of evidence that need explaining.

- First, why do some chemicals react faster than others, when all other variables except the type of chemical are controlled?
  For example, why does magnesium react faster than zinc with hydrochloric acid?

- Second, why do some reactions require an initial input of external energy to react?
  For example, why is a match needed to start the combustion of a hydrocarbon?

B. Activation Energy http://www.youtube.com/watch?v=VbIaK6PLrRM

(An energy barrier that must be overcome for a chemical reaction to occur.)
Entities must reach this minimum energy before they can react. The input energy (which supplies the activation energy) may be in the form of heat, light, or electricity.



The minimum kinetic energy required is analogous to the ***activation energy*** for a reaction. If the ball does not have enough kinetic energy, it will not reach the top of the track and will just roll back to **point A.** This is like two molecules colliding without enough energy to rearrange their bonds - they just rebound elastically.

A ball that returns to **point A** will have the same kinetic energy it began with, but a ball that makes it to **point B** will have more kinetic energy (but less potential energy) because it will be moving faster.

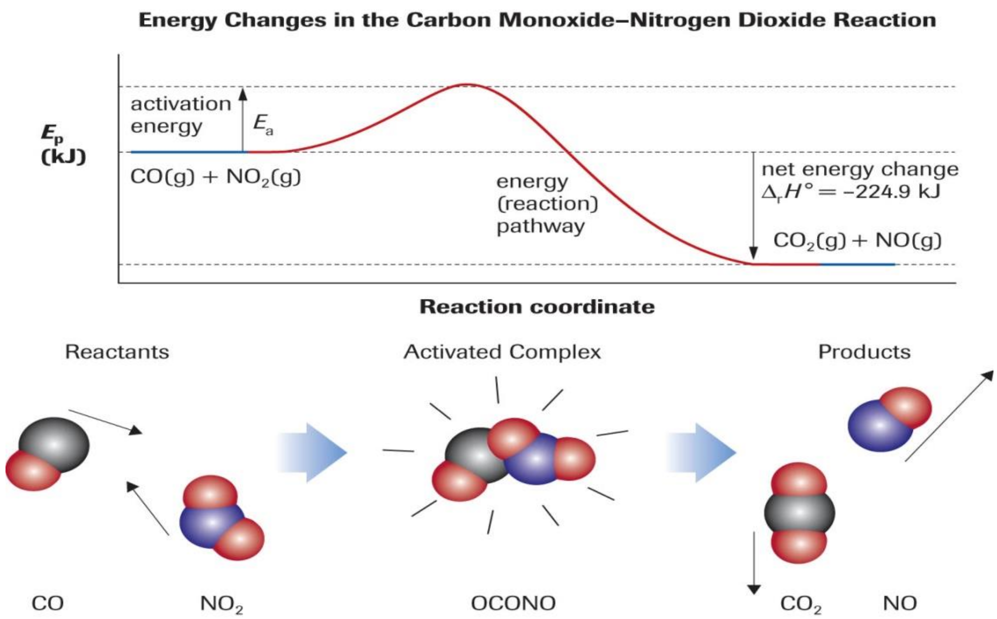
The example above is also analogous to the enthalpy change for an exothermic reaction. The enthalpy change (net chemical energy change) results in energy being immediately released to neighbouring entities.

These entities then move faster, collide with more energy, and are more likely to react.

Exothermic reactions, once begun, often drive themselves.

Consider the reaction of carbon monoxide with nitrogen dioxide, plotted as potential energy of the molecules versus progress of reaction: $CO_{(g)} + NO_{2(g)} \rightarrow CO_{2(g)} + NO_{(g)}$ $\blacktriangle_{r}H^{\circ} = -224.9$ kJ

The molecular collision follows an energy (or reaction) pathway along the plot from left to right.



The ***energy pathway*** is the relative potential energy of the chemical system as it moves from reactants through activated complex to products.

The ***activated complex*** is the chemical entity containing the collided reactants. As the molecules approach each other, they are affected by repulsion forces and begin to slow down. If the molecules have enough kinetic energy, meaning more energy than is required to get to the energy level of the activated complex - they can approach closely enough for their bond structure to rearrange.

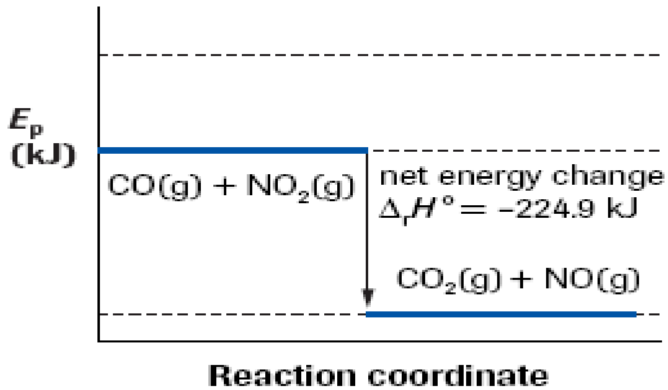
Repulsion forces push the product molecules apart, converting E_P to E_K.

If a large quantity of energy is needed to start a reaction and if the reaction progresses relatively slowly, then the **activation energy is large**.

A spontaneous reaction at room temperature and a higher rate of reaction is interpreted as a relatively **small activation energy**.

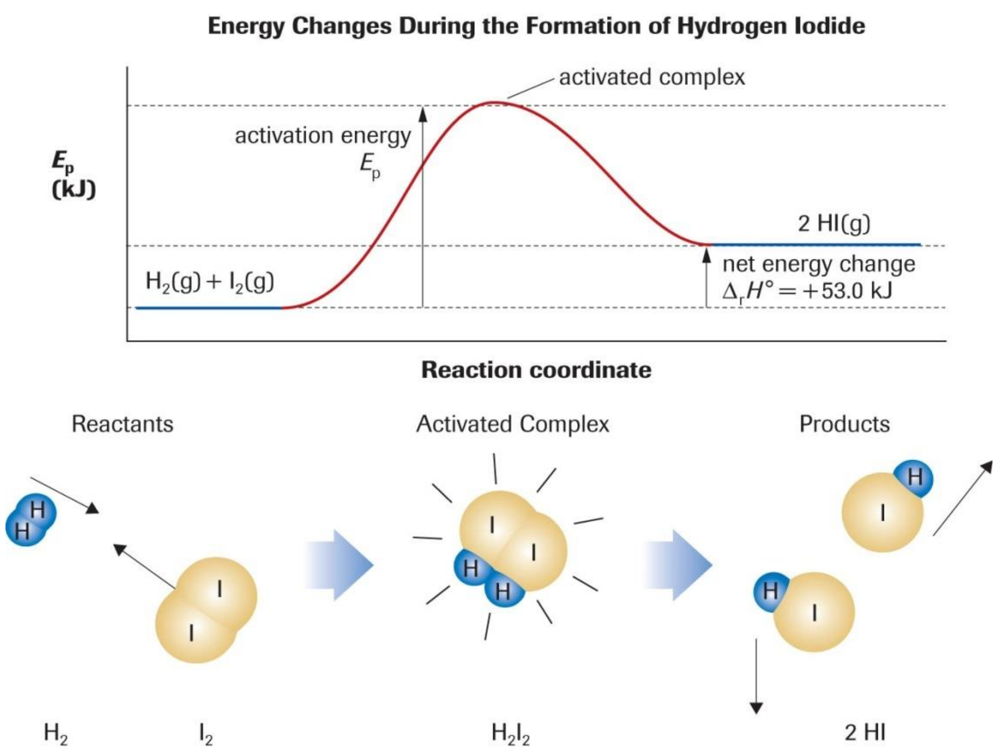
You can think of the new energy pathway diagrams as being an expanded form of **chemical potential energy diagram**, with the approximate energy of the activated complex also represented. This is shown in the following diagram.

Potential Energy (E_p) Diagram Not Including Energy of Activated Complex



Endothermic reactions require a constant input of energy to drive them.

If the potential energy of the products were greater than that of the reactants - the reaction would be endothermic.



A continuous input of energy, usually heat, would be needed to keep the reaction going, and the enthalpy change would be positive.

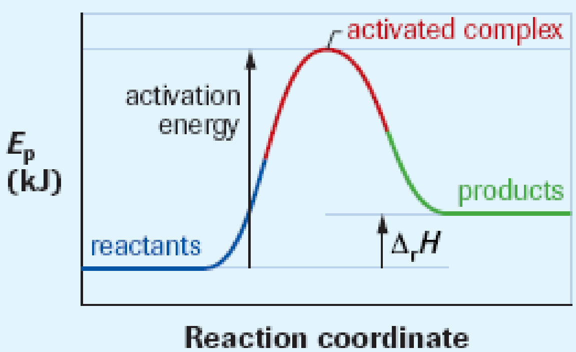
http://www.mhhe.com/physsci/chemistry/essentialchemistry/flash/activa2.swf

COMMUNICATION example

Draw energy pathway diagrams for a general endothermic and a general exothermic reaction. Label the reactants, products, enthalpy change, activation energy, and activated complex.

Solution

Potential Energy Changes During an Endothermic Reaction



Potential Energy Changes During an Exothermic Reaction