Chemical Threats
Advanced Chemistry Course

SAND2010-3899P

Chemical Concepts, Part 3

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

BIOSECURITY ENGAGEMENT PROGRAM

International BIOLOGICAL THREAT REDUCTION

Introduction to Chemistry

- **Chemical Reactions**
  - Thermodynamics
  - Kinetics
  - Equilibrium
  - Catalysts

Thermodynamics/Kinetics

Why is this important?

- Is the chemical reaction favorable?
- What is the energy barrier to producing the products?
- How long is this going to take?
- Can I do anything to speed this up and/or use less energy to get to my desired products?

Chemical Thermodynamics

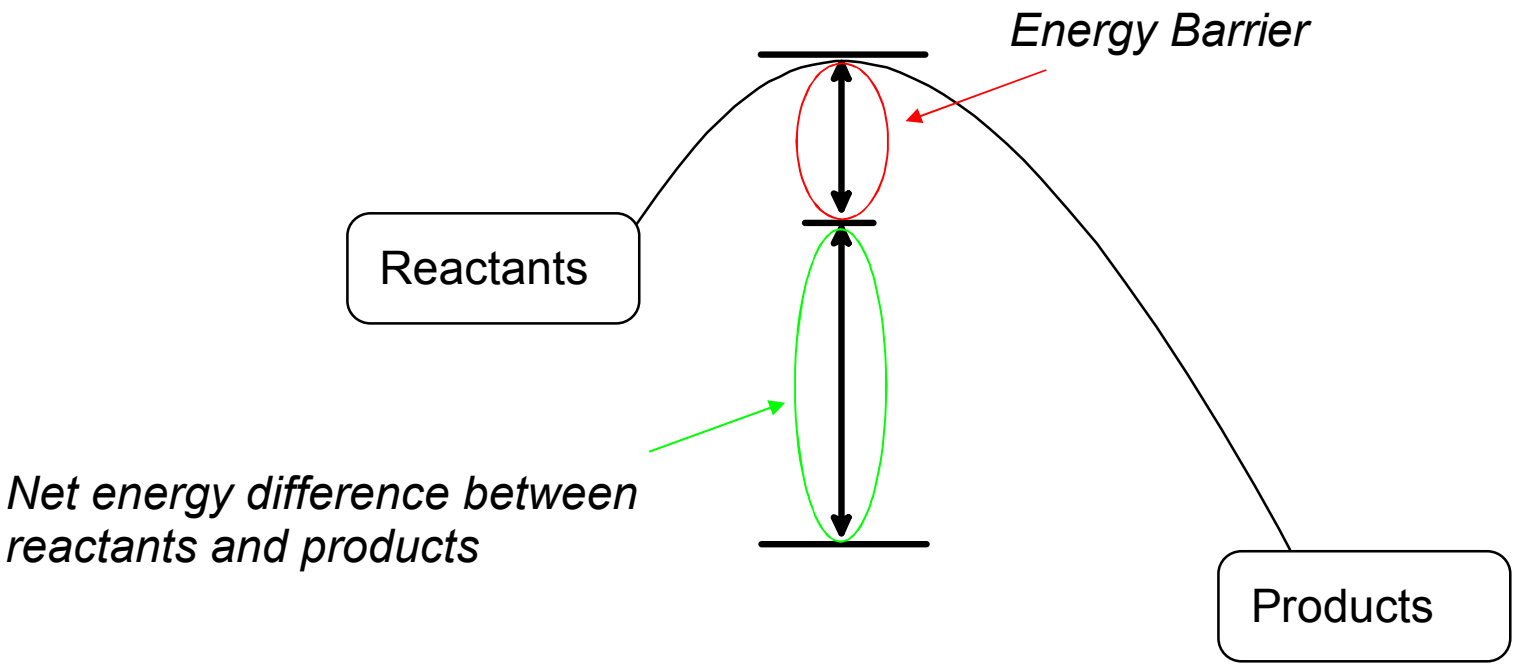
Chemical Thermodynamics is the study of the interrelation of heat and work with

- chemical reactions, or
- physical changes of state

Or, why doesn't this chemical reaction spontaneously occur even if the products are favored?

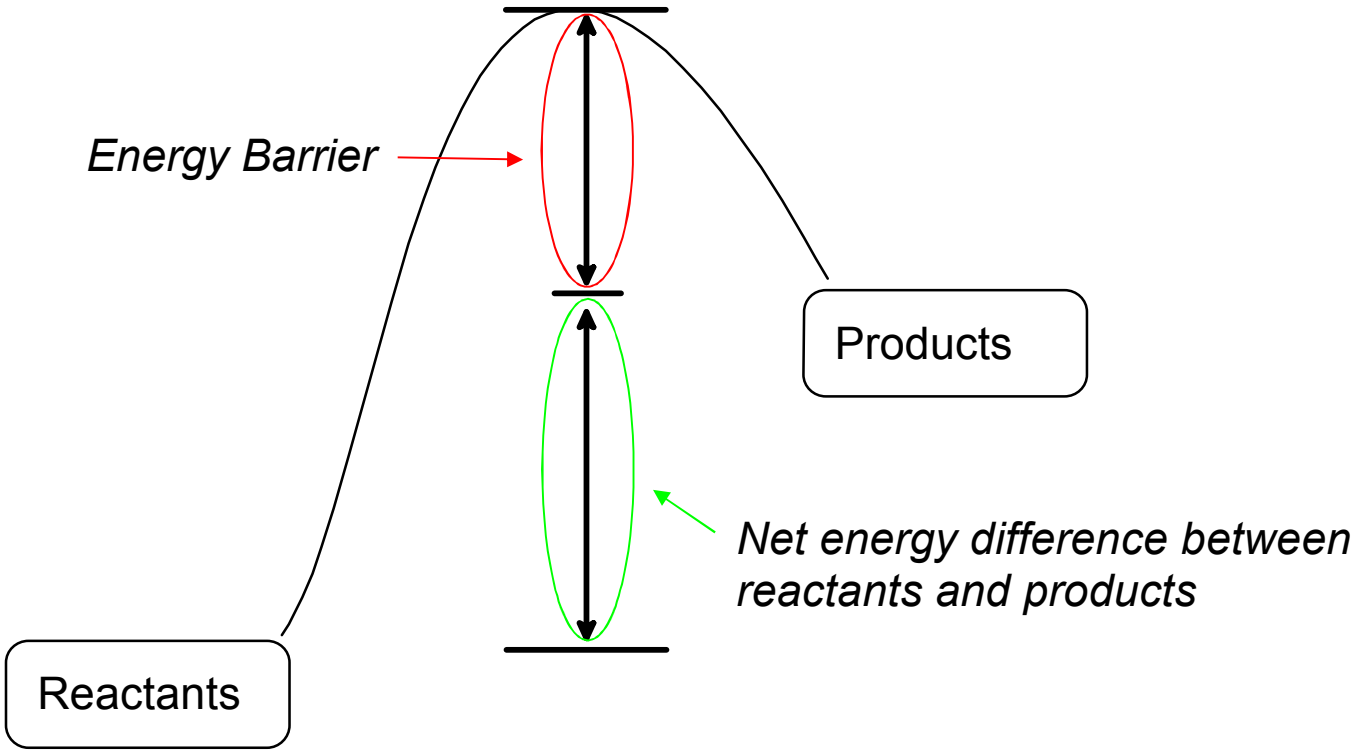
Exothermic Reactions

Exothermic Reactions: Produce heat during the reaction process.



Endothermic Reactions

Endothermic Reactions: Require heat during the reaction process.



Kinetics

Even reactions that are energetically favorable do not happen spontaneously.

$$\text{Rate} = \frac{\text{Change in Concentration}}{\text{Change in Time}}$$

Influenced by:

- Concentration of Reactants
- Temperature

Equilibrium

For the reaction in a sealed container:

At 850°C

$$CaCO_3 \longrightarrow CaO + CO_2$$

When the concentration of carbon dioxide gets high enough.

$$CaO + CO_2 \longrightarrow CaCO_3$$

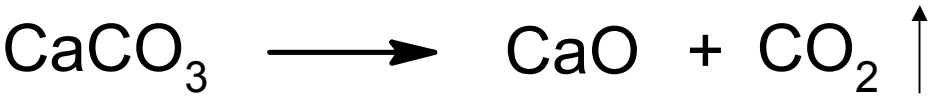
$$CaCO_3 \rightleftharpoons CaO + CO_2$$

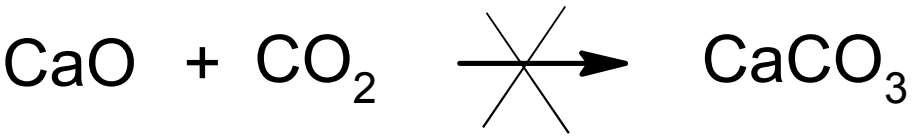
Equilibrium!

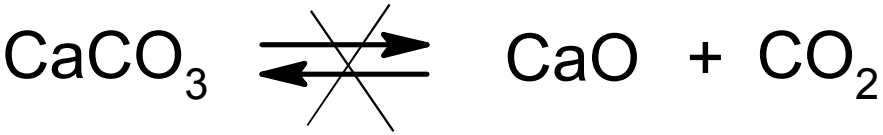
Reactions may be <u>slowed</u> or <u>stopped</u> by the buildup of products.

Equilibrium

If we remove one of the products, there would be no build up of products for the reverse reaction to occur.



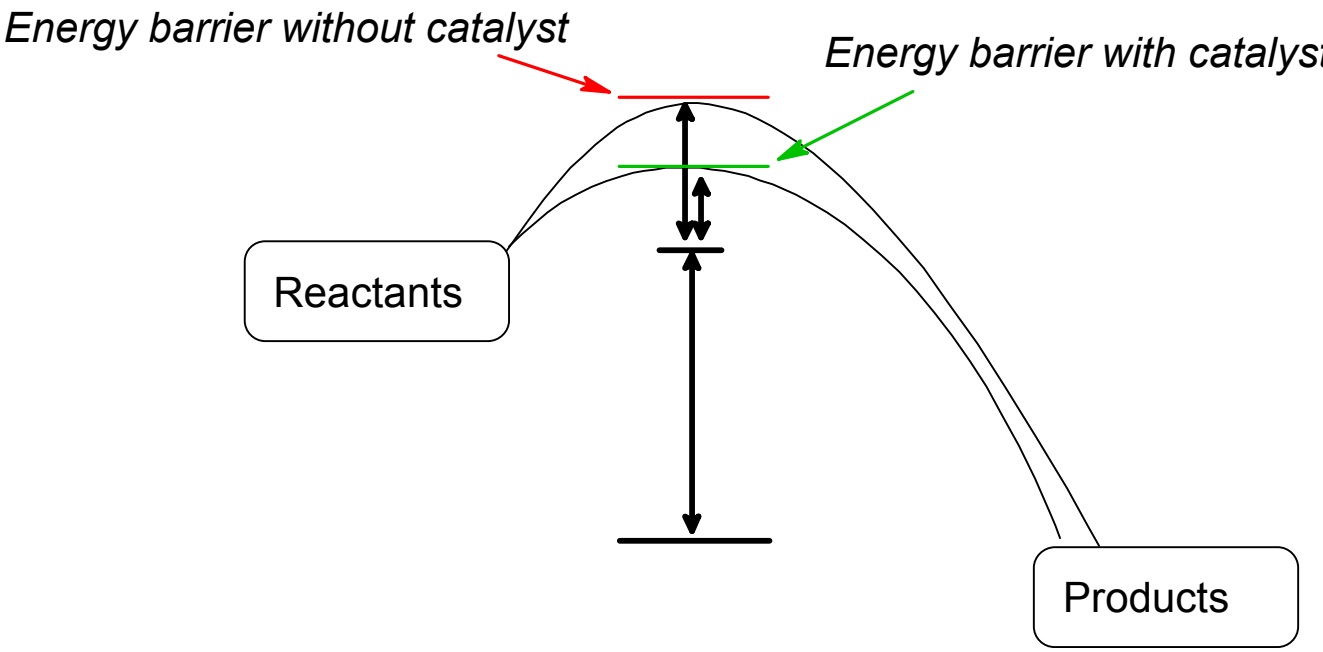




Nonequilibrium condition.

Catalysts

Catalysts: Participate in the reaction by lowering the energy barrier.



Catalysts are not consumed by the reaction.

Summary

- All chemical reactions require some energy input to surmount the 'energy barrier.'
  - **Catalysts lower the energy barrier.**
- Chemical reactions proceed at their own base.
- We can manipulate chemical equilibrium to produce more products.