REACTION RATES AND EQUILIBRIUM

(Ch. 18Sec1) REACTION RATES

--reaction rate - time it takes to form products
--chemical bonding takes place
--The more particles collide, the more kinetic energy the particles have and the higher the probability of product formation. (Collision Theory) - ex: p. 542- squares

(p. 543) Activation E or E_A - minimum amount of E for colliding particles to react
Peak of E_A - activated complex or transition state
(atoms will become molecular or ionic compound)

Reaction Rates are affected by:

I. Temperature - increase in T will speed up the reaction and vice versa.
ex. charcoal burns and releases CO_2 (it has overcome the activation E barrier)
2. Concentration - increase in conc. (# of particles colliding) will increase rate.
3. Particle size - the smaller the particle size, the large the surface area which causes an increase in collisions. Therefore, the reaction rate increases.
4. Catalysts - speeds up reactions; they provide a lower E_A than normal.
Inhibitors interfere with the catalyst by reacting with the catalyst itself. It reduces the amount of catalyst (mold inhibitor)

ex: How do refrigerators prevent food from spoiling?
The kinetic energy of reactants is reduced; fewer particles possess sufficient energy to react.

(Sec 2-p. 549) Reversible Reactions and Equilibrium

Chemical equilibrium -When the rates of the forward and reverse reactions are equal, the reaction has reached a state of balance. Not net change occurs in the actual amounts of the components of the system (chemical reaction).
Dynamic: Forward and reverse reactions occur at the same rate

REVERSIBLE REACTIONS - products and reactants form simultaneously

$$2SO_2(g) + O_2 \text{ --------> } 2\,SO_3\,(g)$$

- Reactants become products at 1st; then as concentration of products build up, the products go back to being reactants.

- Then, as reactants are used up, their concentration decreases. This FORWARD reactions slows down. Eventually, products are forming reactants at the same rate as reactants are forming products.

EQUILIBRIUM POSITION: given by relative concentration of products and reactants at equilibrium.
ex. A ----------> B
1% <---- 99%
(products favored)

In theory, almost all reactions are reversible to come extent under the right conditions. However, in practice, reactants or products are favored at equilibrium.
No LeChatelier's Principle...

EQUILIBRIUM CONSTANTS -p. 556

The position of equilibrium can be expressed by this general expression:

$$aA + bB \rightleftharpoons cC + dD$$

lower case letters - # of moles
[ ] = conc.

K_{eq} = equilibrium constant;

$$\frac{[\text{concentration of products}]^{\text{mol}}}{[\text{concentration of reactants}]^{\text{mol}}}$$

$$K_{eq} = \frac{[C]^c \times [D]^d}{[A]^a \times [B]^b}$$

$K_{eq} > 1$ products favored at equilibrium
$K_{eq} < 1$ reactants favored at equilibrium

ex: The reversible reaction

$N_{(g)} + 3H_{(g)} \rightleftharpoons 2NH_{3(s)}$

produces ammonia, which is a fertilizer. At equilibrium, a 1 L flask contains 0.15 mol of hydrogen, 0.25 mol of nitrogen, and 0.10 mol ammonia. Calculate K_{eq}.

ENTROPY and FREE ENERGY (Ch. 18 Sec. 4) and ENTHALPY (Ch. 17 Sec)

What 2 energy factors determine the course of a reaction?
Entropy (LAW OF DISORDER- matter will scatter spontaneously in a state of chaos!)and **Enthalpy** (Heat)

Free Energy - Energy that is available to do work. Free energy is available to do work, but sometimes it is not efficient. Ex: Car engines are about 30% efficient; only about 30% of the free energy released by burning gasoline is used to propel the car. 70% is lost as friction and waste heat. No process can be made 100% efficient!

- A spontaneous reaction occurs naturally and favors the formation of products at specified conditions. It produces substantial amounts of products at equilibrium and release free energy. A nonspontaneous reaction doesn't favor the formation of products an do not produce substantial amounts of products at equilibrium.

- Many non-spontaneous reactions are required for plants to grow. Nonspontaneous reactions can occur when they are coupled with spontaneous reactions. Photosynthesis is a non-spontaneous one (p. 568). What is another requirement?

  Answer: The combustion of glucose to produce carbon dioxide and water. This reversible reaction is the overall process of photosynthesis, the process by which plants make glucose using CO_2 and H_2O. The free energy value is +2868 kJ/mol. It is non-spontaneous under ordinary conditions.

ENTROPY (S) - p. 568

The disorder of a system.

Entropy is high - marbles scatter
Entropy is low - marbles in a pack

Some guidelines to determine high or low entropy:
I. S, L, G
---------->
increase in entropy

2. # of product molecules > # of reactant molecules
Therefore entropy is high

3. ↑ T, ↑ Entropy

ENTHALPY (H) - (Ch 17 Sec 2: pp. 511-513)

Amount of heat that a substance has at a given T and P.

- *Thermochemistry* - generation or possession of heat.

exothermic reaction - system releases heat its surroundings (combustion)

endothermic - the system absorbs heat from its surroundings (cold pack)

To find out if a chemical reaction will be spontaneous, then heats of formation are used. (p.530)
$\Delta \mathbf{H}_f^\circ$ = standard enthalpy (heat of formation)
ΔH for a reaction is where 1 mol of a compound is formed from its elements.

Under conditions of STP, ΔH for a reaction is:

$$\Delta H = \Delta H_f^\circ \text{(products)} - \Delta H_f^\circ \text{ (reactants)}$$

(exo is a negative value and endo is a positive value)
The more negative, the more stable the compound.

Examples:
$C(s) + O_2(g) \text{ ------> } CO_2(g) \quad \Delta H = -393.5 \text{ kJ}$

$CaCO_3(s) \text{----------> } CaO(s) + CO_2(g) \qquad \Delta H = 176 \text{ kJ}$

NOTE: The above equation is balanced 1,1,1. If other coefficients need to be used, you must multiply them by the S°.
SUMMARY OF ENTHALPY AND ENTROPY effect spontaneity (refer to table) - p. 571& 572

GIBBS FREE ENERGY
This is the maximum amount of energy that can be couple to another process to do useful work.

$\Delta G = \Delta H - T\Delta S$
All spontaneous reactions release free energy. The value of ΔG is NEGATIVE in spontaneous processes because the system loses free energy. Nonspontaneous reactions require that work by expended, so ΔG is positive.

Note- Nonspontaneous reactions under one set of conditions can be spontaneous under another set of conditions.
ex: p. 573 - the effect of T on the decomposition of calcium carbonate

PROGRESS OF CHEMICAL REACTIONS p. 575

The rate of a reaction depends in part on concentrations of the reactants.

Reaction Mechanism - step of elementary reactions
Intermediate - "middle steps" ; the product formed becomes a reactant for the next reaction.