

Chapter 17

Thermodynamics

Thermodynamics

- Study of energy changes in chemical reactions
 - ◆ useful to understand the nature of chemical changes
- Recall thermochemistry (study of heat changes) from Chapter 8
- You are responsible for information from CHM 151, specifically sections 2, 5, 7, 9, and 10 (except "work").

Thermochemistry Review

- 1st Law of Thermodynamics: Energy is conserved, it cannot be created or destroyed
 - ◆ If a system gives off heat, the universe must absorb it (and vice versa).
 - ◆ Heat flow (enthalpy, ΔH) always defined with reference to the system
 - System absorbs heat, $\Delta H > 0$, endothermic
 - System gives off heat, $\Delta H < 0$, exothermic

Calculating $\Delta H^\circ_{\text{rxn}}$

- $\Delta H^\circ_{\text{rxn}} = \sum \Delta H^\circ_f \text{ products} - \sum \Delta H^\circ_f \text{ reactants}$
 - ◆ Heat of formation values, Appendix B
 - ◆ ΔH°_f is reported as kJ/mol
- The $^\circ$ symbol refers to the standard state, 1.00 atm pressure, 25.0°C, 1.00 M for solutions
- Review heat of formation reactions (making 1 mole of substance from its elements in the standard state); Section 8.10
 - ◆ ΔH°_f for elements is 0 (no energy needed!)
- Write heat of formation rxns for $\text{MgCl}_2(\text{s})$ & $\text{H}_2\text{O}(\text{l})$.

Thermodynamics

- How do we know if a chemical reaction will occur?
- How can we tell how far a reaction will go (not how fast, just how far toward products)?
- **Thermodynamics** helps to answer these questions.
- Enthalpy is only one part of the equation.
- Entropy is another.

Spontaneous Processes

- In chemistry, we define a spontaneous process as one that proceeds on its own without any external influence.
 - ◆ Consider the expansion of a gas into a vacuum. This happens spontaneously. The reverse process does not!

• Figure 16.1

Spontaneous Chemical Reactions

- Spontaneous processes
 - ◆ hot object cools
 - ◆ gases expand
 - ◆ iron rusts
 - ◆ Cs reacts with H_2O
- What do all these processes have in common?
- They happen with no external intervention.
 - ◆ Nature tends toward lower energy! **Usually** exothermic reactions are spontaneous (but not always)!!

Spontaneous Processes

- Spontaneous does not mean the same thing as "fast"
 - ◆ Rusting of iron is slow but spontaneous
- Thermodynamics just tells us whether or not a reaction will occur, not how fast it will occur
 - ◆ Kinetics (Ch. 12) looks at that!
- Problem 16.1

Entropy (S)

- Section 8.13: Nature tends toward disorder (increase in entropy).
 - ◆ Who wants to play 52 card pick-up?
- Entropy is a measure of disorder or randomness.
 - ◆ A process is usually spontaneous if it increases the disorder (change in entropy is positive: $\Delta S > 0$)
 - ◆ Units of Entropy (S): Joules/Kelvin (J/K)

Which has the greater entropy?

- Solid, liquid or gas? (ice, water, or steam)

Solid Liquid Gas

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Solid Liquid Gas

Enthalpy & Entropy: ΔH & ΔS

S (s) < S (l) < S (g), Section 10.4

Melting:
 $\Delta H ?$, $\Delta S ?$

Boiling:
 $\Delta H ?$, $\Delta S ?$

Problem 10.7

Which has the greater entropy?

- Solute and solvent or solution?
- Solution has more arrangements, more motion
- Section 11.2

$\text{NaCl(s)} + \text{H}_2\text{O(l)}$ $\text{Na}^+\text{(aq)} + \text{Cl}^-\text{(aq)}$

Which has the greater entropy?

- Low temperature or high temperature?
- Consider gases at different temperatures
- High T: more motion, more possible arrangements
- Figure 16.7

Higher temperature (more disorder) Lower temperature (less disorder)

Group Work

- Which has the greater entropy, separate gases or mixture of gases? Compare numbers of particles.

N_2 O_2 air ($\text{N}_2 + \text{O}_2$)

Which has the greater entropy?

- Reactants or products formed from them?

$$\text{N}_2(\text{g}) + \text{O}_2(\text{g}) \rightleftharpoons 2\text{NO}(\text{g})$$

- The compound has more arrangements even though the same number of molecules are present.
- Worked example 16.1, 16.2; Problem 16.2, 16.3

Which has greater entropy?

- Figure 16.4

Which has greater entropy?

- Worked Key Concept 16.2

Which has greater entropy?

- Key Concept Problem 16.3

Entropy Summary

- Phase changes
 - Boiling: $\Delta H > 0, \Delta S > 0$
 - Melting: $\Delta H > 0, \Delta S > 0$
- Salts dissolving
 - $\Delta H < \text{or} > 0$ (depends), $\Delta S > 0$ (usually)
- Temperature changes
 - Increase: $\Delta S > 0$, more energy, more positions, more possible arrangements
- Skip Section 16.3 (Entropy and probability)

Changes in Entropy

- Does entropy increase or decrease for the following?
 - $2\text{SO}_2(\text{g}) + \text{O}_2(\text{g}) \rightleftharpoons 2\text{SO}_3(\text{g})$
 - $2\text{O}_3(\text{g}) \rightleftharpoons 3\text{O}_2(\text{g})$
 - $\text{CaCO}_3(\text{s}) + 2\text{HCl}(\text{aq}) \rightleftharpoons \text{CaCl}_2(\text{aq}) + \text{H}_2\text{O}(\text{l}) + \text{CO}_2(\text{g})$
 - $\text{C}_2\text{H}_4(\text{g}) + \text{H}_2(\text{g}) \rightleftharpoons \text{CH}_3\text{CH}_3(\text{g})$
 - $\text{NaCl}(\text{s}) \rightarrow \text{Na}^+(\text{aq}) + \text{Cl}^-(\text{aq})$
- More motion, more arrangements for the substances that have more particles
- Worked example 8.11, Problem 8.21, 8.22

Spontaneity

- Which tendency for spontaneity predominates, enthalpy or entropy?
 - They can oppose one another, or they can work together.
- For example, freezing of water at -10°C is exothermic and spontaneous, even though $\Delta S < 0$.
- If we change the entropy of the system, we also change the surroundings, so we must consider the total entropy change.

What makes a process spontaneous?

- Tendency to go to a state of lower energy.
 - Enthalpy: $\Delta H < 0$ (exothermic), but can be endothermic
- Tendency to become more disordered or random
 - Entropy: $\Delta S > 0$ (increase in randomness)
- Randomness increases when particles become further apart.
- Spontaneous: $\Delta H < 0, \Delta S > 0$**
- Non-spontaneous: $\Delta H > 0, \Delta S < 0$**

Entropy and Temperature

- 3rd Law of Thermodynamics: The entropy of a perfectly ordered crystalline substance at 0 K is zero.
- This allows us to calculate S values and changes in entropy (ΔS)
- We can calculate S values and ΔS values; unlike enthalpy - can only measure **change!**
- Use Standard Molar Entropies (Table 16.1) - entropy of 1 mole of a pure substance at 1 atm pressure and 25°C (J/mol·K)
 - Calculate like $\Delta H^\circ_{\text{rxn}}$ (products - reactants)

Standard Molar Entropies

- Notice which phases have lowest values? Highest?

TABLE 16.1 Standard Molar Entropies for Some Common Substances at 25°C					
Substance	Formula	S° (J/K·mol)	Substance	Formula	S° (J/K·mol)
Gases					
Acetylene	C ₂ H ₂	200.9	Acetic acid	CH ₃ COOH	160
Ammonia	NH ₃	192.3	Ethanol	C ₂ H ₅ OH	160
Carbon dioxide	CO ₂	213.6	Methanol	CH ₃ OH	127
Carbon monoxide	CO	191.6	Water	H ₂ O	69.9
Ethylene	C ₂ H ₄	219.9	Solids		
Hydrogen	H ₂	130.6	Calcium carbonate	CaCO ₃	92.9
Methane	CH ₄	186.2	Calcium oxide	CaO	99.7
Nitrogen	N ₂	191.5	Diamond	C	2.4
Nitrogen dioxide	NO ₂	240.0	Graphite	C	5.7
Oxygen	O ₂	205.0	Iron	Fe	27.3
Oxygen (atomic)	O	205.0	Iron(III) oxide	Fe ₂ O ₃	87.4

- Predict and calculate ΔS° for the combustion of methanol.

Entropy Changes

- Calculate $\Delta S^\circ_{\text{rxn}}$ for:
 - $2\text{Na}(\text{s}) + \text{Cl}_2(\text{g}) \rightleftharpoons 2\text{NaCl}(\text{s})$
 - $\text{Na}(\text{s}) = 51.05 \text{ J/mol}\cdot\text{K}, \text{Cl}_2(\text{g}) = 223.0 \text{ J/mol}\cdot\text{K}, \text{NaCl}(\text{s}) = 72.38 \text{ J/mol}\cdot\text{K}$
 - $\Delta S^\circ_{\text{rxn}} = [2(\text{NaCl}(\text{s}))] - [2\text{Na}(\text{s}) + \text{Cl}_2(\text{g})]$
- Not spontaneous with respect to entropy.
- Worked example 16.3, Problem 16.5

Group Work

S° in J/mol K	
H ₂	130.57
O ₂	205.03
H ₂ O(g)	188.71
H ₂ O(l)	69.91

- Calculate ΔS° for the following two reactions:
 - $2\text{H}_2(\text{g}) + \text{O}_2(\text{g}) \rightleftharpoons 2\text{H}_2\text{O}(\text{g})$
 - $2\text{H}_2(\text{g}) + \text{O}_2(\text{g}) \rightleftharpoons 2\text{H}_2\text{O}(\text{l})$
- $\Delta S^\circ = 2S^\circ_{\text{H}_2\text{O}} - 2S^\circ_{\text{H}_2} - S^\circ_{\text{O}_2}$
- Gaseous water: $\Delta S^\circ = -88.75 \text{ J/K}$
 - If we ignore coefficients, = -146.89 (error)
- Liquid water: $\Delta S^\circ = -326.35 \text{ J/K}$

Entropy, 2nd Law of Thermo.

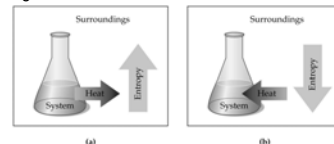
- **2nd Law of Thermodynamics:** in any spontaneous process, the *total* entropy of a system and its surroundings always increases.
 - ◆ The system is the chemical reaction itself.
- ΔS_{tot} is positive for a spontaneous process; ΔS_{tot} is 0 at equilibrium
 - ◆ $\Delta S_{\text{tot}} = \Delta S_{\text{system}} + \Delta S_{\text{surroundings}}$

Entropy

- $\Delta S_{\text{total}} = \Delta S_{\text{system}} + \Delta S_{\text{surroundings}}$
- $\Delta S_{\text{total}} > 0$, the reaction is spontaneous
- $\Delta S_{\text{total}} < 0$, the reaction is nonspontaneous
- $\Delta S_{\text{total}} = 0$, the reaction is at equilibrium
- All reactions proceed spontaneously in a direction that increases the entropy of the system plus the surroundings.

2nd Law of Thermodynamics

- We know how to calculate ΔS_{system} (previous calculations); now calculate ΔS_{surr}
- Figure 16.9



Calculating ΔS_{surr}

- Exothermic: heat leaves system, enters surroundings, surroundings have more energy which gives them more disorder ($\Delta S_{\text{surr}} > 0$ when exothermic: $\Delta H < 0$)
- Endothermic: heat enters system, leaves surroundings, surroundings have less energy which gives them more order ($\Delta S_{\text{surr}} < 0$ when endothermic: $\Delta H > 0$)
- $\Delta S_{\text{surr}} \propto -\Delta H_{\text{rxn}}$ and $\Delta S_{\text{surr}} \propto 1/T$
- Therefore: $\Delta S_{\text{surr}} = -\Delta H_{\text{rxn}}/T$

2nd Law of Thermodynamics

- Calculate ΔS_{tot} for $2\text{CuO}(s) \rightarrow 2\text{Cu}(s) + \text{O}_2(g)$ at 25°C.
- Find $\Delta S_{\text{sys}}^{\circ}$ using molar entropy values.
- Find $\Delta H_{\text{rxn}}^{\circ}$ using standard enthalpy values.
- Find $\Delta S_{\text{surr}}^{\circ}$ using $\Delta H_{\text{rxn}}^{\circ}$ and T.
- $\Delta S_{\text{tot}} = (184.6 \text{ J/K}) + (-1042 \text{ J/K}) = -857 \text{ J/K}$
- Not spontaneous!
- Entropy increased! But what about enthalpy? Also part of the equation.
- Worked Example 16.4, Problem 16.6

Free Energy

- Go Back to Section 8.14
- Gibbs Free Energy Change (ΔG)
 - ◆ Takes into account enthalpy and entropy to predict spontaneity of a reaction.
- $\Delta G = \Delta H - T\Delta S$ (ΔG in units of kJ/mol)
 - ◆ ΔH is enthalpy (kJ/mol)
 - ◆ T is temperature (K)
 - ◆ ΔS is change in entropy (J/mol·K)

Change in Gibbs Free Energy

- Exothermic reactions ($\Delta H < 0$) tend to be spontaneous.
- Increases in entropy ($\Delta S > 0$) tend to be spontaneous.
- What will the sign of ΔG be under these conditions?
 - ◆ $\Delta G = \Delta H - T\Delta S$

Change in Gibbs Free Energy

- Gibbs free energy change or free energy change = ΔG ; maximum amount of energy available to do work on the surroundings
- ΔE or ΔH : some energy is used to do work within the system (rearrange particles, new bonds, ...) and the rest is available to do work on the surroundings (ΔG)
- $\Delta G < 0 \rightarrow$ Spontaneous process
- $\Delta G > 0 \rightarrow$ Nonspontaneous process
- $\Delta G = 0 \rightarrow$ Process is at equilibrium

Free Energy

- Notice that the $T\Delta S$ term is temperature dependent. Temperature plays a part in predicting spontaneity.
 - ◆ For endothermic processes, they are spontaneous at higher temps ($T\Delta S > \Delta H$)
 - ◆ For exothermic processes, they are spontaneous at lower temps ($T\Delta S < \Delta H$)

Free Energy

TABLE 17.2 Signs of Enthalpy, Entropy, and Free-Energy Changes and Reaction Spontaneity for a Reaction at Constant Temperature and Pressure

ΔH	ΔS	$\Delta G = \Delta H - T\Delta S$	Reaction Spontaneity
-	+	-	Spontaneous at all temperatures
-	-	- or +	Spontaneous at low temperatures where ΔH outweighs $T\Delta S$
+	+	- or +	Nonspontaneous at high temperatures where $T\Delta S$ outweighs ΔH
+	-	+	Nonspontaneous at all temperatures
+	+	- or +	Spontaneous at high temperatures where $T\Delta S$ outweighs ΔH
			Nonspontaneous at low temperatures where ΔH outweighs $T\Delta S$

Free Energy

- Using $\Delta G = \Delta H - T\Delta S$, we can predict the sign of ΔG from the sign of ΔH and ΔS .
 - If ΔH is negative and ΔS is positive, ΔG will always be negative.
 - If both ΔH and ΔS are negative, ΔG will be negative only when the temperature value is small.
 - If ΔH is positive and ΔS is negative, ΔG will always be positive.
 - If both ΔH and ΔS are positive, ΔG will be negative only when the temperature value is large.

Decomposition of CuO(s)

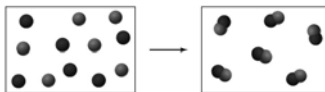
- $2\text{CuO}(s) \rightleftharpoons 2\text{Cu}(s) + \text{O}_2(g)$
 - $\Delta H_{\text{rxn}}^\circ = +310.4 \text{ kJ}$
 - $\Delta S_{\text{rxn}}^\circ = +184.6 \text{ J/K}$
- At room temperature (300 K), is the reaction spontaneous or nonspontaneous?
- At what temperature will the reaction become spontaneous? Temperatures **above** this occur spontaneously because it's endothermic.
- Worked Examples 8.12-13, 16.5; Problems 8.23-8.25, 16.7-16.9

Free Energy and Spontaneity

- Calculate the temperature at which the reaction of nitrogen and chlorine becomes spontaneous. $\Delta H = 460 \text{ kJ}$; $\Delta S = -275 \text{ J/K}$

Key Concept Problem 16.9

- What are the signs (+, -, or 0) of ΔH , ΔS , and ΔG for the following spontaneous reaction of A atoms (red) and B atoms (blue)?



Entropy of Phase Changes

- Phase changes occur at equilibrium ($\Delta G = 0$)
 - $\text{H}_2\text{O}(s) \rightleftharpoons \text{H}_2\text{O}(l)$
 - Solid and liquid are in equilibrium
 - Review phase diagrams from Section 10.11
 - $\Delta G = \Delta H - T\Delta S = 0$, solving for temperature tells us the boiling point!
- Work through Worked Example 10.4 (p. 368)
- Melting Ice:
 - 10°C, 263K: $\Delta G = 6.01 \text{ kJ/mol} - \{263\text{K}\}(0.0220 \text{ kJ/K}\cdot\text{mol}) = +0.22 \text{ kJ/mol}$
 - 0°C, 273K: $\Delta G = 6.01 \text{ kJ/mol} - \{273\text{K}\}(0.0220 \text{ kJ/K}\cdot\text{mol}) = 0.00 \text{ kJ/mol}$
 - +10°C, 283K: $\Delta G = 6.01 \text{ kJ/mol} - \{283\text{K}\}(0.0220 \text{ kJ/K}\cdot\text{mol}) = -0.22 \text{ kJ/mol}$

Phase Change Calculations

- Calculate the boiling point of ethanol if entropy of vaporization is 111.9 J/K and $\Delta H_{\text{vap}} = 39.3 \text{ kJ}$
- Watch units!

Group Work

- $\Delta H = -227 \text{ kJ}$, $\Delta S = -309 \text{ J/K}$, $T = 1450 \text{ K}$. Is this process spontaneous?
- Calculate the temperature (in °C) at which this reaction becomes spontaneous.

Standard Free Energy Changes

- The free energy of a substance depends on temperature, pressure, and physical states (like enthalpy and entropy). We must look at standard-state conditions:
 - Solids, liquids, gases: pure form at 1 atm
 - Solutions at 1 M concentration, gases at 1 atm
 - Room temperature: 25°C (298 K)
- Standard free energy change (ΔG°) is free energy change with reactants and products in their standard states.

Standard Free Energy

- $\Delta G^\circ_{\text{rxn}}$ tells us whether a reaction will favor reactants or products.
 - ◆ $\Delta G^\circ_{\text{rxn}} > 0$: reactant favored. Is K_c large or small?
 - ◆ $\Delta G^\circ_{\text{rxn}} < 0$: product favored. Is K_c large or small?
- Use $\Delta H^\circ_{\text{rxn}}$ and $\Delta S^\circ_{\text{rxn}}$ values to calculate $\Delta G^\circ_{\text{rxn}}$. (We've already done this!)

Standard Free Energy Changes

- Can get ΔG° from $\Delta G^\circ = \Delta H^\circ - T\Delta S^\circ$
 - ◆ Use ΔG° to predict spontaneity in the standard state
- Can also get values of ΔG° from free energies of formation: ΔG°_f (formation from the elements)
- $\Delta G^\circ_f = 0$ for an element in its stable form
 - ◆ This should look familiar (ΔH°_f)
- What are the characteristics of a formation reaction?
 - ◆ 1 mole of product formed
 - ◆ Reactants are elements in standard state.

ΔG°_f

- Which one of these reactions corresponds to ΔG°_f of $\text{H}_2\text{O}(\text{g})$?
 - $2\text{H}_2(\text{g}) + \text{O}_2(\text{g}) \rightleftharpoons 2\text{H}_2\text{O}(\text{g})$
 - $\text{H}_2(\text{g}) + \frac{1}{2}\text{O}_2(\text{g}) \rightleftharpoons \text{H}_2\text{O}(\text{g})$
 - $\text{H}_2(\text{g}) + \frac{1}{2}\text{O}_2(\text{s}) \rightleftharpoons \text{H}_2\text{O}(\text{g})$
- $\Delta G^\circ = \sum n \Delta G^\circ_f \text{ products} - \sum n \Delta G^\circ_f \text{ reactants}$

ΔG°_f

- $\Delta G^\circ = \sum n \Delta G^\circ_f \text{ products} - \sum n \Delta G^\circ_f \text{ reactants}$
- Similarly,
 - $\Delta H^\circ = \sum n \Delta H^\circ_f \text{ products} - \sum n \Delta H^\circ_f \text{ reactants}$
 - $\Delta S^\circ = \sum n S^\circ \text{ products} - \sum n S^\circ \text{ reactants}$
- Values of ΔG°_f , ΔH°_f , S° are listed for standard state conditions in Table 16.3 and Appendix B
- Can use tables to predict the value of ΔG° and the spontaneity of chemical reactions, even ones that have not yet been observed.

Group Work

	ΔG°_f in kJ/mol
CaO(s)	-604.20
Ca(OH) ₂ (s)	-896.76
H ₂	0.00
H ₂ O(g)	-228.59
H ₂ O(l)	-237.18
O ₂	0.00

- Calculate ΔG° and spontaneity for these reactions:
 - $2\text{H}_2(\text{g}) + \text{O}_2(\text{g}) \rightleftharpoons 2\text{H}_2\text{O}(\text{g})$
 - $\text{CaO}(\text{s}) + \text{H}_2\text{O}(\text{l}) \rightleftharpoons \text{Ca}(\text{OH})_2(\text{s})$
- Example 16.7, Problem 16.12

Relating ΔG° to ΔG and K

- ΔG is not standard. It changes as a chemical reaction proceeds, as concentrations and/or temperatures change.
- ΔG° **IS** standard and does **NOT** change during a reaction.
 - $\Delta G = \Delta G^\circ + RT \ln Q$
 - Q (from Ch. 13 - not necessarily at equil.)
 - RT ln Q is correction for non-standard condition; R = 8.314 J/mol·K (unit conversions from 0.08206 L·atm/mol·K)

ΔG and ΔG°

- Consider: $\text{N}_2(\text{g}) + 3\text{H}_2(\text{g}) \rightleftharpoons 2\text{NH}_3(\text{g})$
- $Q_p = (\text{P}_{\text{NH}_3})^2 / [(\text{P}_{\text{N}_2})(\text{P}_{\text{H}_2})^3]$
- If system is at equilibrium, $\Delta G = 0$ and $Q_p = K_p$
 - ◆ $\Delta G^\circ = -RT \ln K$
- If the reaction mixture is mostly reactants:
 - ◆ $Q \ll 1$, $RT \ln Q \ll 0$
 - ◆ $\Delta G < 0$
- If the reaction mixture is mostly products:
 - ◆ $Q \gg 1$, $RT \ln Q \gg 0$
 - ◆ $\Delta G > 0$

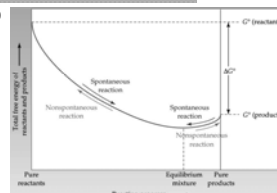
ΔG° and Equilibrium

- $\text{CO}(\text{g}) + \text{H}_2\text{O}(\text{g}) \rightleftharpoons \text{CO}_2(\text{g}) + \text{H}_2(\text{g})$
- $Q = \text{P}_{\text{CO}_2} \text{P}_{\text{H}_2} / \text{P}_{\text{CO}} \text{P}_{\text{H}_2\text{O}}$
- Initially, $Q = 0$, but then it increases
- As the reaction progresses, ΔG decreases until a minimum value of G is reached; at this point, $\Delta G = 0$ and net reaction ceases (though equilibrium is still dynamic; reactants and products still oscillating).

ΔG° and Equilibrium

Figure 16.10

Kotz: 20m09an1
20m09an2



ΔG° and Equilibrium

- When $\Delta G = 0 = \Delta G^\circ + RT \ln Q$, we call this a state of equilibrium.
- At equilibrium, $Q = K$.
- Thus, $\Delta G^\circ = -RT \ln K$
- $\Delta G^\circ > 0$ when $K \ll 1$ (lies toward reactants)
- $\Delta G^\circ < 0$ when $K \gg 1$ (lies toward products)
- $\Delta G^\circ = 0$ when $K = 1$ (roughly equal amounts of reactants and products)
- See Table 16.4

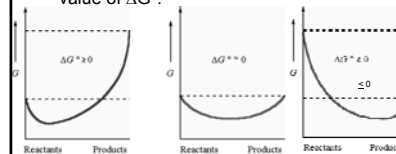
ΔG° and K

TABLE 17.4 Relationship Between the Standard Free-Energy Change and the Equilibrium Constant for a Reaction: $\Delta G^\circ = -RT \ln K$

ΔG°	$\ln K$	K	Comment
$\Delta G^\circ < 0$	$\ln K > 0$	$K > 1$	The equilibrium mixture is mainly products.
$\Delta G^\circ > 0$	$\ln K < 0$	$K < 1$	The equilibrium mixture is mainly reactants.
$\Delta G^\circ = 0$	$\ln K = 0$	$K = 1$	The equilibrium mixture contains comparable amounts of reactants and products ($K = 1$ for 1 M concentrations and 1 atm partial pressures).

ΔG° and Equilibrium

- The position of equilibrium depends on the value of ΔG° .



Calculating K

- $\Delta G^\circ_{\text{rxn}}$ for the formation of ethanol is -24.7 kJ.
- $\text{CO(g)} + 2 \text{H}_2\text{(g)} \rightleftharpoons \text{CH}_3\text{OH(g)}$
- Calculate the equilibrium constant, K , at 25°C for this reaction.
- $\ln K = \Delta G^\circ / -RT$

Calculations Practice

- Calculate K for $2\text{CuO(s)} \rightleftharpoons 2\text{Cu(s)} + \text{O}_2\text{(g)}$ at 25°C.
- Calculate ΔG° from Appendix B values.
 - ◆ $\Delta G^\circ_f(\text{CuO(s)}) = -130 \text{ kJ/mol}$; $\Delta G^\circ_f(\text{Cu(s)}) = 0$;
 - ◆ $\Delta G^\circ_f(\text{O}_2\text{(g)}) = 0$

Calculations Practice

- Calculate ΔG° for $\text{CH}_3\text{COOH(aq)} \rightleftharpoons \text{H}_3\text{O}^+\text{(aq)} + \text{CH}_3\text{COO}^-\text{(aq)}$
- This is a weak acid solution. Find ΔG° at 25°C.
 - ◆ $K_a = 1.8 \times 10^{-5}$

Calculations Practice

- Calculate ΔG for $\text{S(s)} + \text{O}_2\text{(g)} \rightleftharpoons \text{SO}_2\text{(g)}$ when $P_{\text{O}_2} = 0.140 \text{ atm}$ and $P_{\text{SO}_2} = 1.24 \text{ atm}$ at 25°C.
- Need to calculate ΔG° and Q .
 - ◆ $\Delta G^\circ_f(\text{S(s)}) = 0 \text{ kJ/mol}$; $\Delta G^\circ_f(\text{O}_2\text{(g)}) = 0 \text{ kJ/mol}$; $\Delta G^\circ_f(\text{SO}_2\text{(g)}) = -300.2 \text{ kJ/mol}$

Calculations Practice

- ΔG° for the reaction $\text{H}_2\text{(g)} + \text{I}_2\text{(g)} \rightleftharpoons 2 \text{HI(g)}$ is 2.60 kJ at 25°C.
- In one experiment, the initial pressures are $P_{\text{H}_2} = 4.26 \text{ atm}$, $P_{\text{I}_2} = 0.024 \text{ atm}$, and $P_{\text{HI}} = 0.23 \text{ atm}$.
- Calculate ΔG and predict the direction that this reaction will proceed.
- Can compare Q & K values to predict.
- Worked Examples 17.8-11, Problems 16.13-17