Entropy, Enthalpy & Gibbs Free Energy
- ▣ Spontaneous process -occurs without outside intervention
  - ▪ may be fast or slow

Entropy (S)

Entropy, S - a measure of randomness or disorder
- ▣ associated with probability (There are more ways for something to be disorganized than organized.)
- ▣ Entropy increases going from a solid to a liquid to a gas.
- ▣ Entropy increases when solutions are formed.
- ▣ Entropy increases in a reaction when more atoms or molecules are formed.
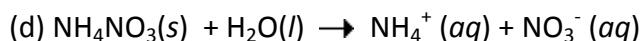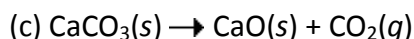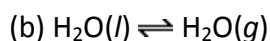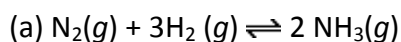- ▣ The entropy of a substance increases with temperature.

2nd Law of Thermodynamics
- ▣ In any spontaneous process there is always an increase in the entropy of the universe.

+ΔS indicates increasing disorder
-ΔS indicates decreasing disorder (becoming more organized)

Which of the following processes will lead to an increase in the entropy of the system?

(a) $N_2(g) + 3H_2 (g) \rightleftharpoons 2 NH_3(g)$

(b) $H_2O(l) \rightleftharpoons H_2O(g)$

(c) $CaCO_3(s) \rightarrow CaO(s) + CO_2(g)$

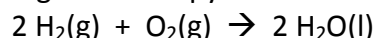(d) $NH_4NO_3(s) + H_2O(l) \rightarrow NH_4^+ (aq) + NO_3^- (aq)$

Enthalpy (H)

- ▣ Remember that we calculate the change in enthalpy (heat) by subtracting the reactants' value from the value of the products.
- ▣ They are given in kilojoules/mol. Remember that the enthalpy of a free element in its standard state is zero.
- ▣ $\Delta H^o = \Sigma \Delta H_f^o{}_{prod} - \Sigma \Delta H_f^o{}_{react}$

+ΔH indicates the reaction is endothermic
-ΔH indicates the reaction is exothermic

EXAMPLE: Calculate the change in enthalpy for the reaction:
$$2 H_2(g) + O_2(g) \rightarrow 2 H_2O(l)$$

Substance	ΔH (kJ/mol)
O_2 (g)	0.00
H_2 (g)	0.00
H_2O (l)	-285.8

Gibbs Free Energy (G)

- ▣ energy available to do work
- ▣ ΔG^o = standard free energy change
  - ■ change in free energy that occurs if the reactants in their standard states are converted to products in their standard states

$$\Delta G^o = \Delta H^o - T\Delta S^o$$

- ▣ A <u>spontaneous reaction has a negative ΔG</u>. For example, when ice melts ΔH is positive (endothermic), ΔS is positive and $\Delta G = 0$ at 0^oC.

+ΔG indicates the reaction is not spontaneous
-ΔG indicates the reaction is spontaneous

- ▣ If...

Entropy, ΔS	Enthalpy, ΔH	Spontaneity
Positive	Positive	Yes at high temp
Negative	Positive	Never spontaneous
Positive	Negative	Always spontaneous
Negative	Negative	Yes at low temp

Ex: Calculate ΔG for a reaction at 25^oC given that the ΔH = -786.1 kJ and ΔS = 0.235 kJ/K.

Is this reaction spontaneous? _____

Is the disorder increasing or decreasing in this reaction? _____

Is the reaction endothermic or exothermic? _____