CONCEPT: GIBBS FREE ENERGY CALCULATIONS

- Gibbs Free Energy formula allows us to calculate the value of _____ (kJ) by using ΔH^o, ΔS^o and T (K) values.
  - □ Note: ΔG^o is under standard conditions while ΔG is under nonstandard conditions.

Gibbs Free Energy Formula

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

- ΔG^o, ΔH^o, ΔS^o = at standard conditions (1 atm, 25°C)

EXAMPLE: For a particular reaction, ΔH^o = - 111.4 kJ and ΔS^o = - 25.0 J/K.

Calculate ΔG^o for this reaction at 298° K. What can be said about the spontaneity of the reaction at this temperature?

a) The system is at equilibrium

b) The system is spontaneous in the reverse direction.

c) The system is spontaneous as written.

Temperature Conditions

- ΔG^o formula can be used to approximate _____ at which reactions are spontaneous or nonspontaneous.
  - □ When ΔG^o value is unknown

EXAMPLE: For the reaction, $N_2(g) + 3\ H_2(g) \rightleftharpoons 2\ NH_3(g)$, ΔH^o = -92.4 kJ, and ΔS^o = -198 J/K. Is the reaction spontaneous under standard conditions? If not at which temperature will it be spontaneous?

STEP 1: Using the Gibbs Free Energy formula, set ΔG^o equal to _____.

- □ Plug in given values for ΔH^o and ΔS^o, and solve for _____.
  - Found temperature corresponds to equilibrium.

STEP 2: Predict spontaneity using _____ of ΔH^o and ΔS^o.

- □ If spontaneous at high temp, reaction will be spontaneous _____ calculated temp.
- □ If spontaneous at low temp, reaction will be spontaneous _____ calculated temp.

Predicting Spontaneity

	+ΔS	-ΔS
+ΔH	**Spontaneous** at HIGH Temperatures	Always nonspontaneous
-ΔH	Always spontaneous	**Spontaneous** at LOW Temperatures

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PRACTICE: Calculate ΔG^o for the following reaction: $P_4\ (s) + 5\ O_2\ (g) \longrightarrow P_4O_{10}\ (s)$, $\Delta H^o = -2940$ kJ/mol, 25ºC.

Does the reaction favor reactants or products?

Substance	S^o (J/mol•K)
P_4 (s)	164.4
O_2 (g)	205.2
P_4O_{10} (g)	228.9

PRACTICE: Determine if reaction is spontaneous under standard conditions, if not at what temperature will it be spontaneous? $3\ A\ (g) + 5\ B\ (s) \longrightarrow 3\ AB\ (s) + B_2\ (g)$ $\Delta H^o = 112.7$ kJ, $\Delta S^o = 78.3$ J/K.

PRACTICE: Nickel has $\Delta H_{vap} = 370.4$ kJ/mol and $\Delta S_{vap} = 123.3$ J/mol•K. Will nickel boil at 2700ºC and 1 atm?

CONCEPT: GIBBS FREE ENERGY CALCULATIONS

Gibbs Free Energy of Reaction

- Similar to ΔS° of reaction formula, ΔG° of reaction can be calculated with free energy of _____.
  - □ These values will always be provided
  - □ Elements in natural state have a Gibbs Free energy of formation equal to _____.

Gibbs Free Energy of Reaction Formula

$$\Delta G^\circ_{rxn} = [\ \sum n G_f^\circ\ (\ \_\_\_\_\_\ )\ -\ \sum n G_f^\circ\ (\ \_\_\_\_\_\ )\ ]$$

- ΔG°_{rxn}= Standard Free Energy of reaction in _____
- $\sum$ = sigma or sum of
- n = _____ of substance
- G_f°= Standard Free Energy of formation in _____

EXAMPLE: Determine ΔG°_{rxn} for the reaction: $HNO_3\,(g) + NH_3\,(g) \longrightarrow NH_4NO_3\,(s)$.

Substance	G°_f (kJ/mol)
HNO_3 (g)	- 73.5
NH_3 (g)	- 16.4
NH_4NO_3 (s)	-183.8

PRACTICE: $Fe_2O_3\,(s) + 3\,H_2\,(g) \longrightarrow 2\,Fe\,(s) + 3\,H_2O\,(g)$ is a redox reaction. What would be its Gibbs Free energy change under standard conditions? Is the reaction spontaneous at 25ºC?

Substance	G°_f (kJ/mol)
Fe_2O_3 (s)	- 742.2
H_2 (g)	0
Fe (s)	0
H_2O (g)	- 228.6