I. Thermochemistry: STUDY OF HEAT IN CHEMICAL REACTIONS AND PHASE CHANGES

A. Heat equation (change in temperature): \[ Q = m \cdot C_p \cdot \Delta T \]
   1. \( Q \) = heat (unit is Joules)
   2. \( m \) = mass (unit is grams)
   3. \( C_p \) = specific heat (unit is J/g\(^\circ\)C)
   4. \( \Delta T \) = temperature (unit is \( ^\circ\)C)
   \( (\Delta T = \text{final temp} - \text{initial temp}) \)

B. Heat equation (phase change): \[ Q = m \cdot H_f \text{ (or } H_v \text{)} \]
   1. \( Q \) = heat (unit is Joules)
   2. \( m \) = mass (unit is grams)
   3. \( H_f \) = heat of fusion (unit is J/g)
   ~ used when phase change occurs between solid \( \leftrightarrow \) liquid
   4. \( H_v \) = heat of vaporization (unit is J/g)
   ~ used when phase change occurs between liquid \( \leftrightarrow \) gas

II. Enthalpy (H): HEAT CONTENT OF A SUBSTANCE

A. Heat of Reaction (\( \Delta H \)):
   AMOUNT OF HEAT ABSORBED OR RELEASED IN A CHEMICAL REACTION

   1. Positive value for \( \Delta H \) means endothermic reaction
   ENDOTHERMIC REACTIONS: Reactants + ENERGY \( \rightarrow \) Products
   ~ Energy is absorbed during the reaction.
   ~ Energy (or heat) is written on left side of the arrow in a chemical equation.
   ~ The heat content of the products is higher than that of the reactants.
   ~ Therefore, the \( \Delta H \) will ALWAYS have a POSITIVE value:
     carbon dioxide + water \( \rightarrow \) sugar + oxygen
     (low heat content) \( \rightarrow \) (high heat content)
   ~ The heat content of sugar and oxygen is much higher than carbon dioxide and water.
   \( \Delta H = H (\text{products}) - H (\text{reactants}) \)
   \( \Delta H = \text{high value} - \text{low value} \)
   \( \text{(sugar & O}_2\text{)} - \text{(CO}_2\text{ & H}_2\text{O)} \)
   \( \Delta H = + \text{(positive) value} \)

   2. Negative value for \( \Delta H \) means exothermic reaction
   EXOTHERMIC REACTIONS: Reactants \( \rightarrow \) Products + ENERGY
   ~ Energy is released during the chemical change.
   ~ Energy (or heat) is written on right side of the arrow in a chemical equation.
   ~ The heat content of the reactants is higher than the heat content of the products.
   ~ Therefore, the \( \Delta H \) will ALWAYS have a NEGATIVE value:
     gasoline + oxygen \( \rightarrow \) carbon dioxide + water
     (high heat content) \( \rightarrow \) (low heat content)
   ~ The heat content of gasoline and oxygen is much higher than carbon dioxide and water.
   \( \Delta H = H (\text{products}) - H (\text{reactants}) \)
   \( \Delta H = \text{low value} - \text{high value} \)
   \( \text{(CO}_2\text{ & H}_2\text{O)} - \text{(gasoline & O}_2\text{)} \)
   \( \Delta H = - \text{(negative) value} \)

III. Entropy (S): DEGREE OF RANDOMNESS OR DISORDER OF THE PARTICLES OF A SUBSTANCE
A. Solids have **low** entropy compared to gases.
B. Gases have **high** entropy compared to solids.

**ENTROPY WORKSHEET**

Entropy is the degree of randomness in a substance. The symbol for change in entropy is $\Delta S$. Solids are very ordered and have low entropy. Liquids and aqueous ions have more entropy because they move about more freely, and gases have an even larger amount of entropy. According to the Second Law of Thermodynamics, *nature is always proceeding to a state of higher entropy.*

Determine whether the following reactions show an increase or decrease in entropy (positive $\Delta S$ or negative $\Delta S$).

1.) $2 \text{KClO}_3 (s) \rightarrow 2 \text{KCl} (s) + 3 \text{O}_2 (g)$
2.) $\text{H}_2\text{O} (l) \rightarrow \text{H}_2\text{O} (s)$
3.) $\text{N}_2 (g) + 3 \text{H}_2 (g) \rightarrow 2 \text{NH}_3 (g)$
4.) $\text{NaCl} (s) \rightarrow \text{Na}^{+1} (aq) + \text{Cl}^{-1} (aq)$
5.) $\text{KCl} (s) \rightarrow \text{KCl} (l)$
6.) $\text{CO}_2 (s) \rightarrow \text{CO}_2 (g)$
7.) $\text{H}^{+1} (aq) + \text{C}_2\text{H}_3\text{O}_2^{-1} (aq) \rightarrow \text{HC}_2\text{H}_3\text{O}_2 (l)$
8.) $\text{C} (s) + \text{O}_2 (g) \rightarrow \text{CO}_2 (g)$
9.) $\text{H}_2 (g) + \text{Cl}_2 (g) \rightarrow 2 \text{HCl} (g)$
10.) $\text{Ag}^{+1} (aq) + \text{Cl}^{-1} (aq) \rightarrow \text{AgCl} (s)$
11.) $2 \text{N}_2\text{O}_5 (g) \rightarrow 4 \text{NO}_2 (g) + \text{O}_2 (g)$
12.) $2 \text{Al} (s) + 3 \text{I}_2 (s) \rightarrow 2 \text{AlI}_3 (s)$
13.) $\text{H}^{+1} (aq) + \text{OH}^{-1} (aq) \rightarrow \text{H}_2\text{O} (l)$
14.) $2 \text{NO} (g) \rightarrow \text{N}_2 (g) + \text{O}_2 (g)$
15.) $\text{H}_2\text{O} (g) \rightarrow \text{H}_2\text{O} (l)$

**UNIT 14 NOTES (CONT’D)**

IV. Gibb’s Free Energy (G)

A. Free energy equation: $\Delta G = \Delta H - T\Delta S$
   1. $\Delta G = \text{CHANGE IN FREE ENERGY}$ (unit is J or kJ)
   2. $\Delta H = \text{HEAT OF REACTION}$ (unit is J or kJ)
   3. $T = \text{TEMPERATURE}$ (unit is Kelvins)
   4. $\Delta S = \text{CHANGE IN ENTROPY}$ (unit is J/K or kJ/K)
B. $\Delta G$ tells whether a reaction occurs spontaneously or not
C. If $\Delta G$ is **negative**, the reaction is spontaneous.

**SPONTANEOUS REACTIONS NOTES**
Some chemical reactions will occur. Some reactions will not occur. What does that mean? Burning paper is a chemical change. Paper + oxygen will produce ashes, smoke, & carbon dioxide gas. That is called a spontaneous reaction. But, can ashes, smoke, & carbon dioxide gas chemically react to form paper? No. That reaction is nonspontaneous; it will not occur.

An iron nail left outside in the rain will rust. That is a spontaneous reaction. But, will a pile of rust turn back into iron? No. That is a nonspontaneous reaction. What determines whether a reaction will or will not occur?

**THERE ARE TWO DRIVING FORCES BEHIND ALL REACTIONS. THOSE FORCES ARE ENTHALPY AND ENTROPY.**

**ENTHALPY:** Reactions tend to move from higher energy to lower energy (exothermic). Enthalpy is calculated and expressed as $\Delta H$.

**ENTROPY:** Reactions tend to move from a highly organized state to a more disorganized state (entropy). Entropy means disorder. Liquids contain more disorder (entropy) than solids. Gases have more disorder (entropy) than liquids or solids. When ice melts, it moves toward more entropy. Entropy is calculated and expressed as $\Delta S$.

**FOR A REACTION TO BE SPONTANEOUS...**
It must either move toward less energy and/or more disorder. (either one or both)

**GIBBS FREE ENERGY WORKSHEET**

The equation for Gibbs Free Energy is:  
$$\Delta G = \Delta H - T\Delta S$$

For a reaction to be spontaneous, the sign for $\Delta G$ has to be negative. $\Delta H$ represents the heat of reaction. $\Delta S$ is the change in entropy. $T$ is temperature in Kelvins.

A negative value for $\Delta H$ means that the reaction is exothermic. That means that heat is released. A positive value for $\Delta H$ means that the reaction is endothermic. That means that heat is absorbed. A negative value for $\Delta S$ means that the products are more ordered than the reactants. A positive value for $\Delta S$ means that the products are less ordered than the reactants.

Part 1 - Complete the following table for the sign of $\Delta G$: $+,-,$ or undetermined. When undetermined, the temperature determines the sign of $\Delta G$.

<table>
<thead>
<tr>
<th>$\Delta H$</th>
<th>$\Delta S$</th>
<th>$\Delta G$</th>
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<tbody>
<tr>
<td>-</td>
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<tr>
<td>+</td>
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</tbody>
</table>

Part 2 - Consider the following reactions. Determine the signs for $\Delta H$ and $\Delta S$. Then decide whether the reaction is sometimes, always, or never spontaneous.

3. $\text{NaOH (s)} \rightarrow \text{Na}^{+1} (\text{aq}) + \text{OH}^{-1} (\text{aq}) + \text{energy}$
   $$\Delta H = _____ \quad \Delta S = _____ \quad \Delta G = _____ \quad \text{________________________ spontaneous}$$
4. \[ \text{energy} + 2 \text{H}_2 (g) + \text{O}_2 (g) \rightarrow \text{H}_2\text{O} (l) \]
\[ \Delta H = _____ \quad \Delta S = _____ \quad \Delta G = _____ \quad \text{spontaneous} \]
5. \[ \text{energy} + \text{H}_2\text{O} (s) \rightarrow \text{H}_2\text{O} (l) \]
\[ \Delta H = _____ \quad \Delta S = _____ \quad \Delta G = _____ \quad \text{spontaneous} \]

Part 4 - Solve the following problems.
6. What is the value of \( \Delta G \) if \( \Delta H = -32.0 \text{ kJ} \), \( \Delta S = +25.0 \text{ kJ/K} \), and \( T = 20 \degree \text{C} \)?
7. Is the reaction described in problem 6 spontaneous?
8. What is the value of \( \Delta G \) if \( \Delta H = +12.0 \text{ kJ} \), \( \Delta S = -5.00 \text{ kJ/K} \), and \( T = 290. \text{ K} \)?
9. Is the reaction described in problem 8 spontaneous?

~ This diagram represents an **exothermic** reaction because overall, heat (energy) is released.

F. Activation energy \( (E_a) \): AMOUNT OF ENERGY REQUIRED TO GET A REACTION STARTED

G. Catalyst: SUBSTANCE THAT SPEEDS UP A CHEMICAL REACTION (BY LOWERING THE ACTIVATION ENERGY) WITHOUT TAKING PART IN THE REACTION

H. An endothermic reaction’s reaction pathway diagram would look like:
A catalyzed reaction would look like:

COLLISION THEORY NOTES (from Modern Chemistry textbook, published by Holt, Rinehart, Winston)
In order for reactions to occur between substances, their particles (molecules, atoms, ions) must collide. Furthermore, their collisions must result in interactions.

The most “effective” collisions produce the fastest reactions. What makes a collision “effective”? -sufficient energy (momentum) -high frequency of collisions -correct orientation of particles

RATE OF REACTIONS NOTES
Rate of reaction: the unit of time required to convert certain amounts of reactants to products; in other words, how fast a reaction will happen

FACTORS INFLUENCING THE RATE OF REACTION:
~ NATURE OF REACTANTS:
- Some substances are just more reactive than others. Iron will oxidize much faster than zinc. Oxygen gas is more reactive than nitrogen gas. (Activity Series & chemical structure)

~ EFFECT OF TEMPERATURE:
- Usually, raising the temperature increases the reaction rate. Increasing temperature increases the kinetic energy and therefore the frequency and the momentum of colliding particles increases.

~ EFFECT OF CONCENTRATION:
- Cramming more particles into a smaller space increases the chance of collisions. Therefore, increasing the concentration of the reactants increases the rate at which a reaction occurs.

~ EFFECT OF PARTICLE SIZE:
- The smaller the particle size, the larger the surface area. Increasing the surface area increases the rate of reaction. Powdered iron filings would rust faster than a solid chunk of iron of the same mass.

~ EFFECT OF CATALYST:
- Catalysts increase the rate of reaction without taking part in the reaction.
ENERGY & CHEMICAL REACTIONS WORKSHEET

1. In your best judgment, which of the following in the pair has the highest entropy?
   A. (A) messy room (B) neat room
   B. (A) ice (B) steam
   C. (A) solid salt crystals (B) salt dissolved in water
   D. (A) iron filings & sulfur powder (B) solid iron sulfide

2. Indicate whether the following describes endothermic or exothermic reactions.
   (A) reactants have higher enthalpy than products
   (B) produces energy as it proceeds
   (C) products have very high enthalpy
   (D) ∆H is always positive
   (E) needs a continuous energy supply as they proceed

3. What is the "direction" or trend most chemical reactions move toward in terms of energy and disorder?

4. What do the following symbols represent:
   (A) ∆H
   (B) ∆S
   (C) ∆G

5. What is the general formula for determining the free energy of a chemical reaction?

6. What does a + ∆G value indicate about a reaction?

7. What does a - ∆G value indicate about a reaction?

8. Match the following:
   ___ + ∆H (A) spontaneous reaction
   ___ - ∆H (B) endothermic reaction
   ___ - ∆G (C) exothermic reaction
   ___ + ∆G (D) nonspontaneous reaction

REACTION PATHWAY DIAGRAM WORKSHEET

Use the following reaction pathway diagram to answer questions 1 – 9.
1. Which of the letters a–f in the diagram represents the potential energy of the products?
2. Which letter indicates the potential energy of the activated complex?
3. Which letter indicates the potential energy of the reactants?
4. Which letter indicates the activation energy of the A + B → C?
5. Which letter indicates the heat of reaction?
6. Is the reaction exothermic or endothermic?
7. Which letter indicates the activation energy of the reverse reaction?
8. Which letter indicates the heat of reaction of the reverse reaction?
9. Is the reverse reaction exothermic or endothermic?

Use the following diagram to answer questions 10 – 21.

10. The heat content of the reactants of the forward reaction is about ______ kilojoules.
11. The heat content of the products of the forward reaction is about ______ kilojoules.
12. The heat content of the activated complex of the forward reaction is about ______ kilojoules.
13. The activation energy of the forward reaction is about ______ kilojoules.
14. The heat of reaction (ΔH) of the forward reaction is about ______ kilojoules.
15. The forward reaction is (endothermic/exothermic).
16. The heat content of the reactants of the reverse reaction is about ______ kilojoules.
17. The heat content of the products of the reverse reaction is about ______ kilojoules.
18. The heat content of the activated complex of the reverse reaction is about ______ kilojoules.
19. The activation energy of the reverse reaction is about ______ kilojoules.
20. The heat of reaction (ΔH) of the reverse reaction is about ______ kilojoules.
21. The reverse reaction is (endothermic/exothermic).

Answer the following questions.
22. Chemical reactions occur when reactants collide. For what reasons may a collision fail to produce a chemical reaction?
23. If every collision between reactants lead to a reaction, what determines the rate at which the reaction occurs?
24. What is the activation energy of a reaction, and how is this energy related to the activated complex of the reaction?
25. What happens when a catalyst is used in a reaction?
26. Name 4 things that will speed up or slow down a chemical reaction.

27. Draw an energy diagram for a reaction. (Label the axes.)

Potential energy of reactants = 350 kJ
Activation energy = 100 kJ
Potential energy of products = 250 kJ

28. Is the reaction in #27 exothermic or endothermic? Explain.

29. How could you lower the activation energy for the reaction in #27?