Name: ____ **Gibbs Free Energy Introduction**

Imagine making plans to hang out with friends. A number of different factors may come into play when deciding what you will do when you meet up. Do you have money to spend? Do you have a means of transportation? What are your available options? These day to day decisions will be used as an analogy for the study of thermodynamics.

1. Using your prior knowledge of chemistry, specifically, enthalpy (heat, ΔH), temperature (kinetic energy, T), and entropy (number of microstates/ randomness, ΔS): For each factor below, explain why each of the corresponding chemical terms and signs (+/-) are analogous.

Factor	Term	Explanation
Money available to spend	**-ΔH**	Reactions release heat like money is released from a bank account.
Money need to save for bills	**+ΔH**	Reactions absorb and store heat like money is saved in an account.
Transportation long distances is available	**High T**	High temperatures increase motion of molecules, like transportation can move people.
Transportation is unavailable or only short distances	**Low T**	Low temperatures restrict particle movement like the inability to transport people.
Endless opportunities, businesses open	**+ΔS**	Increasing entropy increases freedom, like having the freedom to choose plans.
Sunday, businesses are closed	**-ΔS**	Decreasing entropy decreases freedom, like not having the freedom to choose plans.

2. You really need some friend time! Which is more favorable, money available to spend or money needed to save for bills? How is that related to endothermic and exothermic reaction favorability?
   Money to spend is favorable similar to exothermic reactions.

3. Similarly, which is more favorable, endless opportunities for entertainment or businesses being closed? How is that related to entropic favorability?
   Endless opportunities is favorable similar to increasing entropy.

4. Using full sentences:
   a. Explain the best scenario for making plans with your friends including the money, transportation availability, and opportunities.
      Money to spend, transportation, and endless opportunities is the most favorable scenario.

   b. Explain the analogous scenario using thermodynamic terms including enthalpy, temperature, and entropy. Also include the correct sign of each term (+/-).
      Enthalpy is exothermic, temperature is high, and entropy is increasing in the most favorable reaction.

5. The Gibbs free energy is defined as the energy available to do work. If a system is thermodynamically favorable, each factor (enthalpy, temperature, and entropy) play a role. In this analogy, Gibbs free energy may be described as the energy you **release** to go out with your friends (dependent on money, transportation, and opportunities). What algebraic sign would best describe a favorable Gibbs free energy?
   Gibbs free energy values that are favorable are negative (energy is RELEASED)

6. For each scenario, explain how it relates to our analogy for enthalpy, entropy, and thermodynamic favorability. Use signs (+/-) in the small columns. Recall, it would be favorable to go out of the house with your friends.

	Scenario	ΔH°	ΔS°	When will this scenario be favorable? (Always, never, sometimes)
a	You have $200 to spend. You are visiting NYC on a fun Saturday night.	-	+	Always
b	You have $200 to spend. You are grounded.	-	-	Sometimes
c	You are saving money for a school trip. There's a free fair with games, rides, and snacks; but it isn't nearby.	+	+	Sometimes
d	You are saving money for a school trip. You are grounded.	+	-	Never

7. For each scenario is question 6, explain if the availability of free transportation would influence the favorability of the scenario. If so, explain how it would be affected.
   a. Scenario a no effect
   b. Scenario b Decreases favorability (students are taunting with their rides but you aren't allowed to go)
   c. Scenario c Increases favorability due to the ability to arrive at the fair.
   d. Scenario d no effect (still grounded!)

8. For each scenario in question 6, fill in the "Thermodynamic Favorability" column of the table below with + or – for Gibbs free energy. If your answer was "sometimes" based on your answers to question 7 and the analogy of transportation made in question 1, determine if the scenario is more favorable at high or low temperatures.

	Enthalpy, ΔH° (KJ)	Entropy, ΔS° (J)	Thermodynamic Favorability, ΔG (KJ)	Temperature (K) (all T, high T, low T, no T)
a	-	+	-	All
b	-	-	-	Low
c	+	+	-	High
d	+	-	-	All

9. Use complete sentences to explain how changes in enthalpy, temperature, and entropy would create each type of reaction.
   a. A reaction that is always favorable Exothermic reactions with increasing entropy
   b. A reaction that is always unfavorable Endothermic reactions with decreasing entropy
   c. A reaction that is sometimes favorable Exothermic reactions with decreasing entropy OR endothermic reactions with increasing entropy

STOP

10. For each chemical scenario, determine if the reaction is endothermic or exothermic (enthalpy), and whether the reaction is increasing in overall entropy or decreasing. Then decide if the reaction is thermodynamically favorable. If the reaction is temperature dependent, state under which conditions the reaction will be favorable. Use the table created above to guide you.

	Reaction	**Enthalpy (+/-)**	**Entropy (+/-)**	**Favorability (+/-)**
a	$CH_3OH(l) + 3/2\ O_2(g) \rightarrow CO_2(g) + 2H_2O(g)$ + heat	-	+	Always
b	$CO(g) + 2H_2(g) \rightarrow CH_3OH(l)$ + 128.13 kJ/mol	-	-	- if low T
c	177kJ/mol + $CaCO_3(s) \rightarrow CaO(s) + CO_2(g)$	+	+	- if high T
d	49kJ/mol + $6C(s) + 3H_2(g) \rightarrow C_6H_6(l)$	+	-	never

Gibbs Free Energy is calculated using the formula below. The ° symbol means the calculation is for systems at 298K and 1 atmosphere. For each question, calculate the Gibbs free energy to determine if the reaction is thermodynamically favorable.

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

11. The hydrogenation of ethene gas at 298. K shows a decrease in disorder (ΔS° = -120.7 J/(mol•K)) during an exothermic reaction (ΔH° = -136.9 kJ/mol).
    a. Compare the units of enthalpy and entropy and record them below. Before calculating any variable, what must you do to ensure you will have all the units correct?
    Enthalpy is kJ/mol and Entropy is J/molK which implies one of the units will need to be converted (preferably to kJ).
    b. Notice the units of entropy include Kelvin. Why is entropy temperature dependent and multiplied by the temperature of the reaction?
    Entropy is temperature dependent which is why it is multiplied by the Kelvin temperature.

    c. Determine whether the reaction is thermodynamically favorable or nonspontaneous by calculating ΔG°.
    $C_2H_4\ (g) + H_2\ (g) \rightarrow C_2H_6\ (g)$
    X = -136.9 – (298)(0.1207)
    X = -100.9 KJ/mol
    favorable
12. Copper (I) sulfide reacts with sulfur to produce copper (II) sulfide at 25°C. The process is exothermic (ΔH° = -26.7 kJ/mol) with a decrease in disorder (ΔS° = -19.7 J/(mol•K)). Determine the thermodynamic favorablity of the reaction by calculating ΔG°. $Cu_2S\ (s) + S\ (s) \rightarrow 2\ CuS\ (s)$
    X = -26.7 – (298)(-0.0197)
    X= -20.8 kJ/mol
    favorable

Much like enthalpy and entropy, Gibbs free energy is a state function because they describe quantitatively an equilibrium state of a thermodynamic system, irrespective of how the system arrived in that state. Additionally, like enthalpy and entropy, Gibbs free energy can be calculated independently using the equation below.

$$\Delta G_r^\circ = \sum G_f^\circ \text{ products} - \sum G_f^\circ \text{ reactants}$$

13. What is the standard free energy change, ΔG°, in kJ, for the following reaction at 298K?
    $C_2H_5OH(l) + 3O_2(g) \rightarrow 2CO_2(g) + 3H_2O(g)$

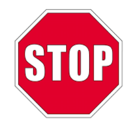
Compound	ΔG_f° $kJ \cdot mol^{-1}$
$C_2H_5OH(l)$	-175
$O_2(g)$	0
$CO_2(g)$	-394
$H_2O(g)$	-229

[2(-394) + 3(-229)] – [-175 + 3(0)]

-1.30×10^3 kJ/mol

Favorable

14. Just because a system is thermodynamically favorable, does not mean a reaction will be observable. What other factor(s) should be considered when observing reactions and explaining if they have a measurable reaction rate? Insufficient activation energy to start the reaction.



Reaction thermodynamic favorability can be tied to equilibrium conditions. Considering the analogy made in the first part of this activity, where you are trying to spend time with your friends. This was dependent on funding, opportunity, and transportation. The "equation" for this could be as described below, where Y stands for You and F stands for Friends.

$$Y + 2F \leftrightarrow YF_2$$

15. Explain the difference between the "reactants" and the "products" of this equation. When are you alone and when are you with your friends?
    Reactants Y + 2F are apart, Products YF2 is when you are "bonding" with your friends.

16. Write the equilibrium constant expression for this scenario assuming all factors affect equilibrium conditions.
    $K = \frac{[YF_2]}{[Y][F]^2}$
17. If the scenario is favorable, will the K value be larger than 1, smaller than 1, or equal to 1?
    K > 1 because [YF2] > [Y] + [2F]
18. If the scenario is unfavorable, will the K value be larger than 1, smaller than 1, or equal to 1?
    K < 1 because [YF2] < [Y] + [2F]
19. Using your answers above, and your new understanding of Gibbs free energy, fill in the summary of how Gibbs free energy, equilibrium constant values, and thermodynamic favorability are related.

ΔG°	K (<,>, or = to 1)	Favorability (yes/no)
+	K<1	No
-	K.1	Yes
0	K=1	equilibrium

20. If a reaction is thermodynamically unfavorable, what shift can be made to create a favorable reaction?
    Reverse the reaction to create a favorable reaction where Gibbs free energy will be calculated in the opposite direction and become negative and K will inverse to become large.