Thermodynamics and Kinetics

Energy

What is Energy?

- Energy is the ability to do work or produce heat

- Chemical Potential Energy- energy stored in a substance because of its composition
  - Type of atoms
  - Arrangement of atoms
  - Number and type of bonds

What is heat?

- Heat (q) is energy that is in the process of flowing from one object to another

- Heat always flows from a warmer object to a cooler object

  - Warmer object loses energy in the form of heat and its temperature decreases
  - Cooler object gains energy in the form of heat and its temperature increases

- NOT THE SAME AS TEMPERATURE

Temperature

- Temperature (T) is the average kinetic energy of the molecules in a substance

Measuring Heat: Two Units

- Calorie (cal)- the amount of heat required to raise the temperature of 1 gram of pure water 1°C.

- Joule (J) SI Unit for heat (1 cal= 4.184joules)

Thermochemistry and Enthalpy

Thermochemistry

- Thermochemistry is the study of heat changes associated with phase changes and chemical reactions

Universe= System + Surroundings

- System- the specific part of the universe that contains the reaction process you wish to study

- Surroundings-everything else

Enthalpy (H)

- Enthalpy (H) is a measure of the heat content of a system at a constant pressure

- Enthalpy of Reaction (ΔH_{rxn})= $H_{products}$- $H_{reactants}$ (or ΔH)

- Thermochemical equations are balanced chemical equations that include values for ΔH

Enthalpy (H)

- Endothermic Reactions
  - Heat is absorbed
  - Heat is treated as a reactant
  - + ΔH

- Exothermic Reactions
  - Heat is released
  - Heat is treated as a product
  - - ΔH

Hess's Law

- If you can add the reactions, you can add the enthalpy changes

- Three Rules
  - If the reaction must be doubled, so must the value of ΔH
  - If the reaction must be reversed, the sign of ΔH must be reversed
  - Anything on both sides of the final equation cancels

Example:

- Calculate the ΔH for the reaction $2S\ (s) + 3O_2 \rightarrow 2SO_3\ (g)$ using the information below.

a. $2SO_3\ (g) \rightarrow 2SO_2\ (g) + O_2\ (g)$ ΔH= 198kJ

b. $S\ (s) + O_2\ (g) \rightarrow SO_2\ (g)$ ΔH= - 297kJ

Desired Reaction Equation: $2S\ (s) + 3O_2 \rightarrow 2SO_3\ (g)$

a. $2SO_3\ (g) \rightarrow 2SO_2\ (g) + O_2\ (g)$ $\Delta H = 198kJ$

b. $S\ (s) + O_2\ (g) \rightarrow SO_2\ (g)$ $\Delta H = -297kJ$

- SO_3 is on the product side of the desired equation so reverse reaction a.

Desired Reaction Equation: $2S (s) + 3O_2 \rightarrow 2SO_3 (g)$

a. $2SO_2 (g) + O_2 (g) \rightarrow 2SO_3 (g)$ $\Delta H = -198 kJ$

b. $S (s) + O_2 (g) \rightarrow SO_2 (g)$ $\Delta H = -297 kJ$

- The coefficient of the 1st reactant, S (s) is 2 in the desired equation. Therefore reaction b must be doubled.

Desired Reaction Equation: $2S (s) + 3O_2 \rightarrow 2SO_3 (g)$

a. $2SO_2 (g) + O_2 (g) \rightarrow 2SO_3 (g)$ ΔH= -198kJ

b. $2S (s) + 2O_2 (g) \rightarrow 2SO_2 (g)$ ΔH= - 594kJ

- Add the equations together and cancel anything that occurs on both the reactant and product side.

Desired Reaction Equation: $2S\ (s) + 3O_2 \rightarrow 2SO_3\ (g)$

$2SO_2\ (g) + 3O_2\ (g) + 2S\ (s) \rightarrow 2SO_2\ (g) + 2SO_3\ (g)$ ΔH= - 792kJ

- Write the final equation for the reaction including the ΔH value. Box or circle.

Spontaneity, Entropy, Enthalpy, and Gibb’s Free Energy

Spontaneity

- Spontaneous processes- physical or chemical changes that occur with no outside intervention

- Nonspontaneous processes- require outside intervention to occur

Can we use enthalpy change to predict spontaneity?

What kind of reactions, endothermic or exothermic, would you predict to be spontaneous?


Entropy (S)

- Entropy is a measure of disorder or randomness of the particles in a system

- 2nd Law of Thermodynamics- all spontaneous processes increase the entropy of the universe

Gibb's Free Energy (G)

- Gibb's free energy is defined as the energy available to do work
- It relates enthalpy and entropy and can be used to predict reaction spontaneity
- Formula for Gibb's Free Energy:

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

- If ΔG value is negative, the reaction is spontaneous
- If ΔG value is positive, the reaction is nonspontanoues

Spontaneity, Enthalpy, and Entropy

	Exothermic Reactions ($-\Delta H$)	Endothermic Reactions ($+\Delta H$)
Increased Entropy ($+\Delta S$)		
Decreased Entropy ($-\Delta S$)		

Specific Heat

Specific Heat (c)

- Specific heat is the amount of heat required to raise the temperature of 1g of a substance 1°C

Substances with High Specific Heat

- Absorb and release more heat
- Have the ability to hold heat longer
- Take more energy transfer (and more time) to heat up or cool down

Substances with Low Specific Heat

- Absorb and release small amounts of heat
- Do not hold heat as long
- Take less energy transfer (and less time) to heat up or cool down

Formula for Heat Transfer

$$q = mc\Delta T$$

- q= heat absorbed or released
  - If the value for q is negative, heat is released from an object
  - If the value for q is positive, heat is absorbed by the object
- m= mass
- c= specific heat (substance specific)
- ΔT= change in temperature ($T_{final} - T_{initial}$)

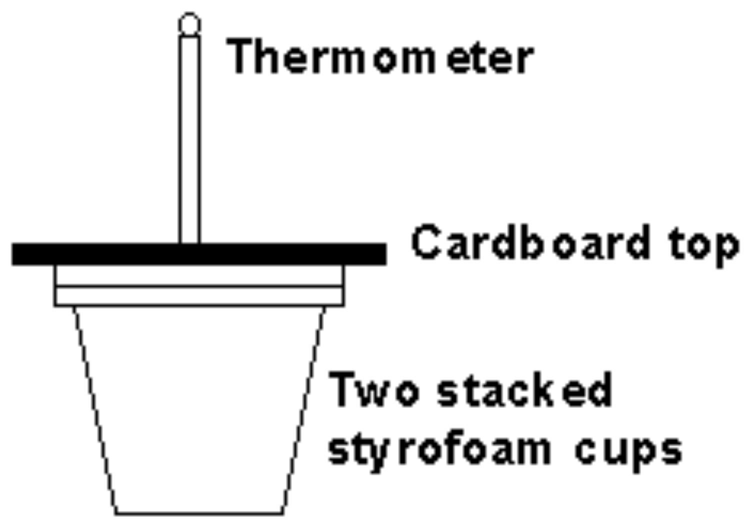
Law of Conservation of Energy

- The law of conservation of energy states that energy (heat) can neither be created nor destroyed, only transferred
- 1^{st} Law of Thermodynamics
- Heat lost by the object in question must be absorbed by the surroundings

-q released= + q absorbed

Calorimeters

- Heat transfer is measured using a device called a calorimeter



Specific Heat Example Problems

Example 1:

- If the temperature of 34.4g of ethanol increases from 25.0°C to 78.8°C, how much heat has been absorbed by the ethanol? (The specific heat of ethanol is 2.44J/g°C)

Example 2:

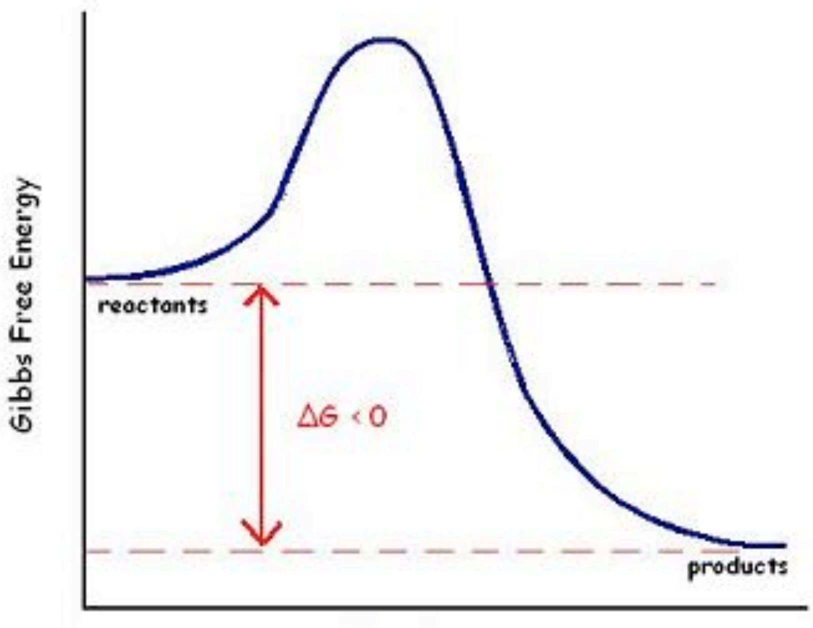
- A 4.50g nugget of pure gold absorbed 267J of heat. What was the final temperature of the gold if the initial temperature was 25°C? (The specific heat of gold is 0.129J/g°C.)

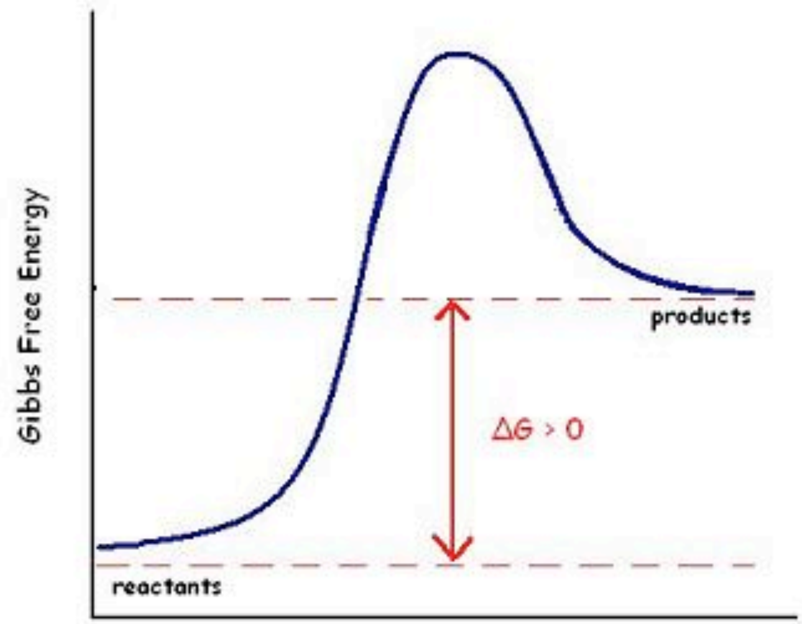
Example 3:

- A 155g sample of an unknown substance was heated from 25.0°C to 40.0°C. In the process, the substance absorbed 5696 J of energy. What is the specific heat of the substance?

Activation Energy and Reaction Rates

Reaction Energy Diagrams





Activation Energy

- Activation energy (E_A) is the minimum amount of energy that reacting particles must have to form an activated complex
- Reaction the activated complex requires collisions in the right orientation
- High Activation energy correlates to a slow reaction rate
- Low activation energy correlates to a fast reaction rate

Factors that Affect Reaction Rates

- Nature of reactants- some elements or compounds are not as reactive as others
- Concentration- greater concentration of reactants leads to more collisions
- Surface Area- greater surface area of reactants (smaller particles) leads to more collisions
- Temperature- increase in temperature= increase in movement= increase in collisions

- Catalysts- lower the activation energy of reactants
  - Example: Enzymes