CHEMISTRY FOR ENGINEERS

Chapter 1: Thermochemistry

Defining Energy

Kinetic Energy - energy in motion

$$KE = \frac{1}{2}mv^2$$

KE - kinetic energy
m - mass of the object
v - velocity of the object

Potential Energy - energy by virtue of an object's position/ elevation

$$PE = mgh$$

PE - potential energy of the body
g - gravitational acceleration (9.81 m/s^2)
h - the object's height/ elevation

Internal energy - combination of the potential and kinetic energies of the atoms and molecules of a substance

Chemical energy **-** energy released in the formation of bonds in a chemical reaction

Radiant energy - energy from light/ electromagnetic radiation

Mechanical energy - energy from the movement of macroscopic objects

Thermal energy - energy that arises from the temperature of an object

Electrical energy - energy that arises from moving charges

Nuclear energy - energy that comes from nuclear fission and fusion processes

Heat (q) **-** flow of energy between two objects due to a thermal difference

Work (w) **-** transfer of energy accomplished by a force moving an object a certain distance against resistance

Pressure - volume (PV) work **-** most common type of work encountered in chemistry

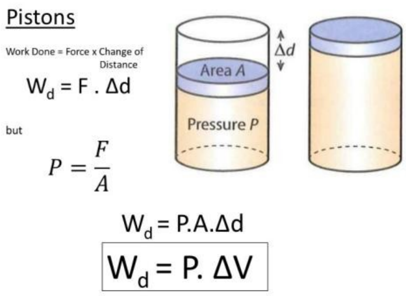
Sample Problems

1. How fast (in meters per second) must an iron ball with a mass of 56.6 g be traveling in order to have a kinetic energy of 15.75 J? The density of iron is 7.87 g/cm^3.

2. What is the potential energy of an object whise mass is 5 kg that is placed 10 m above ground level?

3. The total kinetic energy of a sample's molecules is 100 J. The total potential energy is 50 J. What is its internal energy?

4. How many kJ of work is done if a cylinder's volume decreases by 3.27 L against a constant pressure of 1 atm?



Units of Energy

calorie - amount of energy required to heat one gram of water by 1°C

Joule (J) **-** SI unit of energy defined as 1 kg-m^2/s^2

Calorie (Cal) **-** energy unit in food, defined as 1000 calories

Btu (British thermal unit) **-** amount of energy required to heat one pound of water by 1°F

Conversion: 1 Btu = 252 calories

Energy Transformation and Conservation

System **-** part of the Universe being considered

Surroundings **-** remainder of the Universe being considered

Boundary **-** separation between the system and the surroundings

First Law of Thermodynamics **-** energy can neither be created nor destroyed

$$\Delta E = q + w$$
$$\Delta E = E_{final} - E_{initial}$$

Path properties **-** properties that depend on the path that the system takes to get there. Example: q and w

State properties **-** properties that are independent of the path taken to get there. Example: temperature, volume and enthalpy

State properties
Sample Problems
If a machine does 4.8×10^3 kJ of work after an input of 7.31×10^4 kJ of heat, what is the change in internal energy for the machine?

Heat Capacity and Calorimetry

Calorimetry - observation of heat flow in and out of the system using various techniques

Specific heat capacity - measures the heat required to heat one gram of a material by 1°C

Molar heat capacity - measures the heat required to heat one mole of a material by 1°C

Sample Problem:
1. Heating a 24.0-g aluminum can raises its temperature by 15.0°C. Find the value of q for the can (C_p= 0.9 J/g-°C).

2. The molar heat capacity of liquid water is 75.3 J/mol K. If 37.5 g of water is cooled from 42.0 to 7.0°C, what is q for the water?

3. A glass contains 250.0 g of warm water at 78.0°C. A piece of gold at 2.30°C is placed in the water. The final temperature reached by this system is 76.9°C. What was the mass of gold? The specific heat of water is 4.184 J/g °C, and that of gold is 0.129 J/g °C.

4. A calorimeter is to be used to compare the energy content of some fuels. In the calibration of the calorimeter, an electrical resistance heater supplies 100.0 J of heat and a temperature increase of 0.850°C is observed. Then 0.245 g of a particular fuel is burned in this same calorimeter, and the temperature increases by 5.23°C. Calculate the energy density of this fuel, which is the amount of energy liberated per gram of fuel burned.

Enthalpy - heat absorbed/released as a result of a chemical reaction that occurs at constant pressure

Exothermic **-** heat is evolved from the system

Endothermic - heat is absorbed from the system

Fusion **-** also known as melting, change from the solid phase to the liquid phase

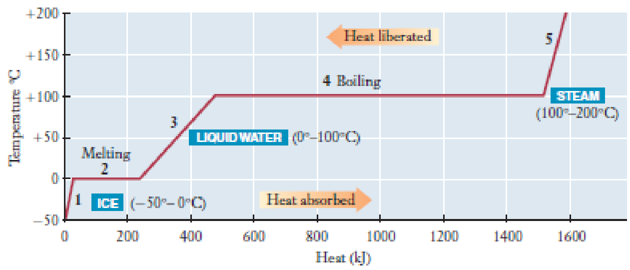
Freezing - change from the liquid phase to the solid phase

Vaporization **-** change from the liquid phase to the vapor phase

Condensation - change from the vapor phase to the liquid phase

Sublimation **-** change from the vapor phase to the solid phase

Deposition **-** change from the solid phase to the vapor phase



For water:
Specific heat of ice = 2.108 kJ/kg-K
Specific heat of water = 4.187 kJ/kg-K
Specific heat of steam = 1.996 kJ/kg-K
Latent heat of fusion = 333.55 kJ/kg
Latent heat of vaporization = 2257 kJ/kg

The total enthalpy change is equal to the sum of the individual enthalpy changes that the sytem undergoes.

Sample Problems:
1. The heat of fusion of pure silicon is 43.4 kJ/mol. How much energy would be needed to melt a 5.24-g sample of silicon at its melting point of 1693 K?

2. ΔH_{vap} = 31.3 kJ/mol for acetone. If 1.40 kg of water were vaporized to steam in a boiler, how much acetone (in kg) would need to be vaporized to use the same amount of heat?

3. Calculate the energy required to convert 1.70 g of ice originally at –12.0°C into steam at 105°C.

Hess' Law and Heats of Reaction

Thermochemical equation **-** summary of the over-all energetics of a chemical reaction

Standard Enthalpy Change for Heat of Formation ($\Delta°H_f$) **-** enthalpy change when one mole of a substance is formed from its elements at standard state

Standard state **-** Substances in their natural phase at physical conditions of 298.15 K and 1 atm

Values for $\Delta°H_f$ can be looked up in tables like this one:

Standard Enthalpies of Formation, ΔH

Substance	Formula	ΔH_f° (kJ/mol)
Acetylene	$C_2H_2(g)$	−26.7
Ammonia	$NH_3(g)$	−46.19
Benzene	$C_6H_6(l)$	49.04
Calcium carbonate	$CaCO_3(s)$	−1207.1
Calcium oxide	$CaO(s)$	−635.5
Carbon dioxide	$CO_2(g)$	−393.5
Carbon monoxide	$CO(g)$	−110.5
Diamond	$C(s)$	1.88
Ethane	$C_2H_6(g)$	−84.68
Ethanol	$C_2H_5OH(l)$	−277.7
Ethylene	$C_2H_4(g)$	52.30
Glucose	$C_6H_{12}O_6(s)$	−1260
Hydrogen bromide	$HBr(g)$	236.23

Hess' Law **-** the enthalpy change for any process is independent of the particular way the process is carried out. Enthalpy is a state property.

$$\Delta H^\circ = \sum_i \nu_i \Delta H_f^\circ\,(\text{product})_i - \sum_j \nu_j \Delta H_f^\circ\,(\text{reactant})_j$$

Rules:
1. The reaction can be reversed. This will change the sign of ΔH_f.
2. The reaction can be multiplied by a constant. The value of ΔH_f must be multiplied by the same constant.
3. Any combination of the first two rules may be used.

Sample Problem:

Using these reactions, find the standard enthalpy change for the formation of 1 mol PbO(s) from lead metal and oxygen gas.

$PbO(s) + C(graphite) \rightarrow Pb(s) + CO(g)$ $\Delta H° = 106.8$ kJ

$2C(graphite) + O_2(g) \rightarrow 2CO(g)$ $\Delta H° = -221.0$ kJ

If 250. g of lead reacts with oxygen to form lead(II) oxide, what quantity of thermal energy (in kJ) is absorbed or evolved?

Energy and Stochiometry

Sample Problem

Nitroglycerine, $C_3H_5(NO_3)_3(l)$, is an explosive most often used in mine or quarry blasting. It is a powerful explosive because four gases (N_2, O_2, CO_2, and steam) are formed when nitroglycerine is detonated. In addition, 6.26 kJ of heat is given off per gram of nitroglycerine detonated.

(a) Write a balanced thermochemical equation for the reaction.

(b) What is ΔH when 4.65 mol of products is formed?

Cumulative Problems

1. A runner generates 418 kJ of energy per kilometer from the cellular oxidation of food. The runner's body must dissipate this heat or the body will overheat. Suppose that sweat evaporation is the only important cooling mechanism. If you estimate the enthalpy of evaporation of water as 44 kJ/mol and assume that sweat can be treated as water,describe how you would estimate the volume of sweat that would have to be evaporated if the runner runs a 10-km race.