Chapter 5: thermochemistry

- thermodynamics – study of energy and its transformations
- thermochemistry – relationships between chemical reactions and energy changes

5.1 The Nature of Energy
- w = Fd
- heat – energy transferred from hotter object to colder one
- energy – capacity to do work

5.1.1 Kinetic and Potential Energy
- kinetic energy – energy of motion

  - $K = \dfrac{1}{2}mv^2$

- potential energy – stored energy
    - electron has potential energy when near a proton
    - charged particles have potential energy through attractive and repulsive electrostatic forces
- chemical energy – potential energy stored in arrangement of atoms
- thermal energy – kinetic energy of molecules

5.1.2 Energy Units
- SI unit for energy = joule, J
- $1J = 1\ kg*m^2/s^2$
- 1cal = 4.184 J
- 1 Cal = 1000cal = 1kcal

5.1.3 Systems and Surroundings
- system – specific amount of matter defined for study
    - surroundings – everything outside of system

5.2 The First Law of Thermodynamics
- first law of thermodynamics – conservation of energy

5.2.1 Internal Energy
- total energy of system – sum of all kinetic and potential energy
- internal energy – total energy of a system

  - $\Delta E = E_{final} + E_{inital}$

  - $+\Delta E -$ system gains energy from surroundings

  - $-\Delta E =$ system loses energy to surroundings

5.2.2 Relating ΔE to Heat and Work
- system can exchange energy in two ways : heat and work
- ΔE = q + w
- both heat added and work done on system increases internal energy
- both heat lost and work done by system on surrounding lower internal energy

Sign Conversion for q:	Sign ΔE = q + w
q>0; heat transferred from surroundings to system	q>0 and w>0; ΔE>0
q<0; heat transferred from system to surroundings	q>0 and w<0; sign depends on magnitudes of q and w
Sign conversion for w:	
w>0; work done by surroundings on system	q<0 and w>0; sign depends on magnitudes of q and w
w<0; work done by system on surroundings	q<0 and w<0; ΔE<0

5.2.3 Endothermic and Exothermic Processes
- endothermic – absorption of heat by system
- exothermic – evolution of heat

5.2.4 State Functions
- state function – property of system determined by specifying its conditions
- value of state function does not depend on particular history of sample only its present conditions
    - E is a state function - ΔE depends only on initial and final states

5.3 Enthalpy
- enthalpy – heat absorbed or released under constant pressure
    - state function
- change in enthalpy equals heat gained or lost by system when process occurs under constant pressure
- $\Delta H = H_{final} - H_{initial} = q_p$
- $+\Delta H$ – system gains heat, endothermic
- $-\Delta H$ – system releases heat, exothermic

5.4 Enthalpies of Reaction
- $\Delta H = H(products) - H(reactants)$
- enthalpy of reaction – energy change in a reaction
- thermochemical equations – balanced equations that show enthalpy change
- guidelines for using thermochemical equations and enthalpy diagrams
    - 1) enthalpy is an extensive property
        - magnitude of ΔH directly proportional to amount of reactant consumed in process
    - 2) enthalpy change for reaction equal in magnitude but opposite in sign to ΔH for reverse reaction
    - 3) enthalpy change for a reaction depends on state of reactants and products

5.5 Calorimetry
- calorimetry – measurement of heat flow
- calorimeter – measures heat flow

5.5.1 Heat Capacity and Specific Heat
- heat capacity – amount of heat required to raise temperature by 1K or 1°C
- molar heat capacity – heat capacity of 1mol of substance
- specific heat – heat capacity of 1g of substance
- $$\text{specific heat} = \frac{\text{quantity of heat transferreed}}{(\text{grams substance}) \times (\text{temp change})} = \frac{q}{m \times \Delta T}$$

5.5.2 Constant Pressure Calorimetry
- $q_{soln} = (\text{specific heat of solution}) \times (\text{grams solution}) \times \Delta T$
- dilute aqueous solutions have specific heats that are the same as water
- $q_{rxn} = -q_{so\ln}$
- temperature increase (+ΔT) – reaction is exothermic (-q$_{rxn}$)

5.5.3 Bomb Calorimeter (constant volume calorimeter)
- bomb calorimeter – used to study combustion in reactions
- $q_{rxn} = -C_{calorimeter} \times \Delta T$
- $C_{calorimeter}$ – heat capacity of calorimeter
    - Because constant volume – heat transferred corresponds to energy change rather than enthalpy change

5.6 Hess's Law

- Hess's Law – if a reaction is carried out in a series of steps, ΔH for the reaction will be equal to the sum of the enthalpy changes for the individual steps
- Always get same value of ΔH for overall reaction, regardless of steps

5.7 Enthalpies of Formation
- enthalpy of formation – enthalpy change from formation of a compound (ΔH_f)
- standard state – 1atm and 298K (25°C)
- standard enthalpy – enthalpy change when reactants and products in standard states ($\Delta H°$)
- standard enthalpy of formation – change in enthalpy for reaction that forms 1mol of compound from elements, with all substances in standard states (ΔH_f°)
- standard enthalpy of formation of most stable form of any element is zero

5.7.1 Using Enthalpies of Formation to Calculate Enthalpies of Reaction
- $$\Delta H_{rxn}^\circ = \Sigma\, n\Delta H_f^\circ \,(\text{products}) \times \Sigma\, m\Delta H_f^\circ \,(\text{reactants})$$
- n, m stoichiometric coefficients of reaction
- first term – formation of reaction of products
- second term – reverse formation reactions of reactants

5.8 Foods and Fuels
- fuel value – energy releases when 1g of material is combusted

5.8.1 Foods
- body uses chemical energy from foods for:
  - maintaining body temperature, drive muscles, construct and repair tissues
- fats serve as body's energy reserve
  - 1) insoluble in water
  - 2) produce more energy per gram
- average fuel value for fat – 38kJ/g (9 kcal/g)
- average fuel value of proteins and carbohydrates – 17kJ/g (4 kcal/g)

5.8.2 Fuels
- the greater then percentage of carbon and hydrogen in a fuel, the higher the fuel value
- fossil fuels – coal, petroleum, natural gas
- natural gas – gaseous hydrocarbons, mostly methane, small amounts of ethane, propane, and butane
- petroleum – mostly hydrocarbons; rest composed of compounds containing sulfur, nitrogen, or oxygen
- coal – hydrocarbons of high molecular weight, and compounds of sulfur, oxygen, and nitrogen
- coal gasification
  - coal + steam → complex mixture → mixture if CH_4, H_2, and CO (syngas)
  - syngas – easier to transport, less air pollution

5.8.3 Other Energy Sources
- nuclear and solar energy