THERMOCHEMISTRY

- ENTHALPIES OF FORMATION
  - <delta>H[f]
  - magnitude of enthalpy change is dependent on
    - temperature
    - pressure
    - state
  - standard state of a substance
    - its pure form at 1 atm and the temperature of interest
    - allows comparisons of different reactions with different states
  - standard enthalpy change
    - enthalpy change when all the reactants and products are in their standard states
    - <delta>H^o
  - standard enthalpy of formation
    - change in enthalpy for the reaction that forms one mole of the compound from its elements with all substances in their standard states
    - the standard enthalpy of formation of the most stable form of any element is zero
  - CALCULATING ENTHALPIES OF REACTION FROM ENTHALPIES OF FORMATION
    - STEPS
      - 1 - decomposition
      - 2 - formation of one product
      - 3 - formation of second product
    - assume the stoichiometric coefficients in the balanced equation represent the number of moles of each substance
    - <delta>H^o[rxn] = <sigma>m<delta>H^o (products) - <sigma>n<delta>H^o (reactants)
      - <sigma>m<delta>H^o (reactants) = sum of enthalpies of formation of reactants
      - <sigma>n<delta>H^o (products) = sum of enthalpies of formation of products
      - n and m = stoichiometric coefficients of the relevant chemical equation
- HESS'S LAW
  - if a reaction is carried out in a series of steps, the change in enthalpy for the overall reaction equals the sum of the enthalpy changes for the individual steps
  - for a particular set of reactants and products, change in enthalpy is the same whether the reaction takes place in one step or in a series of steps
- CALORIMETRY
  - HEAT CAPACITY AND SPECIFIC HEAT
    - heat capacity
      - C
      - the heat required to raise the temperature of an object by 1K (1 degC)
    - molar heat capacity
      - Cm
      - heat capacity of one mole of substance (per substance)
    - specific heat
      - Cs
      - heat capacity of one gram of substance
      - q = Cs X m X <delta>T ⟶ Cs = q/(m<delta>T)
  - CONSTANT-PRESSURE CALORIMETRY
    - system = reactants and products
    - water = part of the surroundings
    - measure temperature change of the water based on the assumption that any heat given off or absorbed goes to or from the water to or from the reaction
    - q[soln] = (specific heat of solution) x (grams of solution) x (temperature change) = -q[rxn]
    - q[rxn] < 0 = exothermic reaction
  - BOMB CALORIMETRY
    - constant volume calorimetry
    - must know the total heat capacity of the calorimeter (Ccal)
    - used for combustion reactions
    - Ccal = q/<delta>T
- ENTHALPIES OF REACTION
  - HEAT OF REACTION
    - <delta>H[rxn]
      - endothermic rxns have a negative value
      - exothermic rxns have a positive value
    - <delta>H = H[products] - H[reactants]
  - ENTHALPY DIAGRAM
  - THERMOCHEMICAL EQUATIONS GUIDELINES
    - enthalpy is an extensive property
      - the magnitude of enthalpy change is proportional to the amount of substance consumed
    - enthalpy change for the reverse reaction is equal magnitude but opposite sign
      - eg. +3 in the forward = -3 in the reverse
    - enthalpy change depends on the states of the reactants and products
- ENTHALPY
  - ENTHALPY
    - relates to heat flow under conditions of constant pressure
      - constant pressure = atmospheric pressure in most reactions
    - H = E + PV
      - H = enthalpy
      - E = internal energy
      - P = pressure of the system
      - V = volume of a system
    - state function
  - PRESSURE-VOLUME WORK
    - work involved in the expansion and compression of gas
    - work done by a chemical reaction is expansion or compression (volume change)
    - when a gas expands a system does work on the surroundings
    - units = L-atm
    - 1 L-atm = 101.3 J
    - work done = -pressure ⟶ w = -P<delta>V
  - ENTHALPY CHANGE
    - change in enthalpy = the heat gained or lost at constant pressure
    - <delta>H = <delta>E + P<delta>V
    - state function
    - <delta>H is positive
      - system gains heat
      - endothermic reaction
    - <delta>H is positive
      - system loses heat
      - exothermic reaction

- ENERGY
  - KINETIC ENERGY AND POTENTIAL ENERGY
    - kinetic energy
      - the energy of motion
      - depends on mass and speed of the object
        - Ek increases as speed increases
        - Ek increases with increase in mass
      - Ek = 1/2(mv^2)
    - potential energy
      - energy possessed by virtue of its position relative to other objects (stored energy)
      - electrostatic potential energy
        - E[p]
        - potential energy arising from the interactions between charged particles
          - E[p] is directly proportional to the electrical charges on the two interacting objects
          - E[p] is indirectly proportional to the distance separating them
        - E[p] = (k)(Q)(Q[2])/d
          - k = proportionality constant ⟶ 8.99 X 10^9 (J-m/C^2)
          - Q1/Q2 = electrical charges of interacting objects
          - d = distance between the objects
  - UNITS OF ENERGY
    - Joule (J)
      - 1J = 1kg-m^2/s^2
      - SI unit
    - calorie (cal)
      - 1 cal = 4.184 J
    - Calorie (Cal)
      - nutritional energy unit
      - 1 Cal = 1 kcal
  - SYSTEM AND SURROUNDINGS
    - division of the universe
      - the system
        - portion singled out for study
        - reactants and products of a chemical reaction
      - the surroundings
        - everything except the system
        - in a chemical lab = container and everything beyond it
    - systems
      - open
        - matter is exchanged with the surroundings
        - energy is exchanged with the surroundings
        - e.g. = unwrapped pot of boiling water on a stove
      - closed
        - matter is not exchanged with the surroundings
        - energy is exchanged with the surroundings
        - e.g. = piston and cylinder such as in a car engine
      - isolated
        - matter is not exchanged with the surroundings
        - energy is not exchanged with the surroundings
        - e.g. = insulated thermos (vacuum)
  - TRANSFERRING ENERGY
    - HEAT ⟶ energy transferred from a hotter object to a colder one
    - WORK ⟶ energy transferred when a force moves an object
      - w
      - the magnitude of work done on the object is the force x the distance the object moves = F x d
  - energy is the capacity to do work or produce heat
- THE FIRST LAW OF THERMODYNAMICS
  - INTERNAL ENERGY
    - internal energy of a system (E) is the sum of all the kinetic and potential energies of the components of the system
    - E has a fixed value for a given set of conditions and is proportional to the total quantity of matter in the system
      - temperature affects internal energy
      - pressure influences internal energy
    - change in internal energy = final internal energy of the system - initial internal energy of the system
      - initial internal energy of the system = internal energy of the reactants
      - final internal energy of the system = internal energy of the products
    - positive value for change in internal energy = energy is gained by the system
    - negative value for change in internal energy = the system has lost energy
  - RELATING CHANGE IN INTERNAL ENERGY TO HEAT AND WORK
    - when heat is added to or work is done on a system, its internal energy increases
    - change in internal energy = sum of the heat added to or liberated from the system and the work done on or by the system
    - <delta>E = q + w
      - q = heat added to or liberated from the system
        - q = + system gains heat
        - q = - system loses heat
      - w = work done by or on the system
        - w = + work done on system
        - w = - work done by system
      - <delta>E = change in internal energy of the system
        - <delta>E = + net gain of energy by system
        - <delta>E = - net loss of energy by system
  - ENDOTHERMIC AND EXOTHERMIC PROCESSES
    - endothermic
      - system absorbs from the surroundings
      - + q value
    - exothermic
      - system releases heat to the surroundings
      - - q value
  - STATE FUNCTIONS
    - the value of a state function depends only on the present state of the system, not on the path it took to reach that state
    - state function is only interested in the change between the initial state and final state of a system
  - THE FIRST LAW
    - energy can neither be created nor destroyed ⟶ energy is conserved
    - energy lost by a system is absorbed by its surroundings and vice versa

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Page 1 of 1

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