Chapter 6: Electronic Structure of Atoms

- **electronic structure** – the arrangement of electrons in an atom

6.1 The Wave Nature of Light

- **electronic radiation** – radiant energy, carries energy through space
- all electromagnetic radiation move through a vacuum at 3.00 x 10^8 m/s
- **wavelength** – the distance between successive peaks in a wave
- **electromagnetic radiation** – 1) electric component
  2) magnetic components
- wave characteristics due to periodic oscillations of the two components
- wavelength and frequency are related
- $\nu\lambda = c$ (ν=wavelength, λ=frequency)
- frequency expressed in cycles per second (hertz, Hz)

Unit	Symbol	Length(m)	Type of Radiation
Angstrom	Å	10^{-10}	X ray
Nanometer	nm	10^{-9}	Ultraviolet, visible
Micrometer	μm	10^{-6}	Infrared
Millimeter	mm	10^{-3}	Infrared
Centimeter	mm	10^{-2}	Microwave
Meter	M	1	TV, radio

6.2 Quantized Energy and Photons

- German physicist, Max Planck – energy can be released by atoms only in "chunks" of some minimum size
- **Quantum** – smallest quantity of energy that can be emitted or absorbed as electromagnetic radiation
- E=hv (h=planck's constant=6.63 x 10^{-34} J-s)

6.2.1 The Photoelectric Effect

- **photoelectric effect** – when photons strike a metal surface, electrons are emitted

6.3 Bohr's Model of the Hydrogen Atom

6.3.1 Line Spectra

- monochromatic – radiation with a single wavelength
- spectrum – created when radiation is divided up into its wavelengths
- continuous wavelength – rainbow of colors containing light of all wavelengths
- line spectrum – spectrum containing radiation of specific wavelengths
- Johann Balmer:
  - $\nu = C(1/2^2 – 1/n^2)$ n = 3,4,5,6
  - C = 3.29 x 10^{15} s^{-1}

6.3.2 Bohr's Model

- electrons could circle the nucleus only orbits of specific radii
- $E_n = (-R_H)(1/n^2)$ n = 1,2,3,4…
- R_H = Rydberg constant = 2.18 x 10^{-18} J
- n = principle quantum number
- gound state – lowest energy level
- excited state – electrons in a higher energy level
- $E_\infty = (-2.18 \times 10^{-18}\ J)(1/\infty^2) = 0$
- Electrons can jump to a higher energy state by absorbing energy
- $\triangle E = E_f – E_I = h\nu$

- n_i and n_f are the principle quantum numbers of the initial and final states of the atom
- ν is positive when $n_i < n_f$ (energy is absorbed)
- ν is negative when $n_i > n_f$ (electron jumps from higher to lower state)
- frequency of electromagnetic radiation must be a positive number
- "-" sign indicates that light is emitted

6.4 The Wave Behavior of Matter

- De Broglie: wavelength of the electron or any particle depends on its mass, m and velocity, v
- $\lambda = h/mv$
- mv = momentum
- matter waves – describe the waves characteristics of material particles

6.4.1 The Uncertainty Principle

- it is impossible to know simultaneously both the exact momentum of the electron and its exact location in space

6.5 Quantum Mechanics and Atomic Orbitals

- **wave functions** - ψ (has no physical meaning)
- **probability density** - ψ^2, probability that the electron will be found at the location proposed
- **electron density** – regions where there is a high probability of finding the electron

6.5.1 Orbitals and Quantum Numbers

- 1) principal quantum number, n, can have integral values of 1,2,3,4…
  - n increases orbital becomes larger
- 2) azimuthal quantum number, l, can have integral values from 0 to n-1
  - defines the shape of the orbital
- 3) magnetic quantum number, m_l, can have integral values between l and –l, and 0
  - describes orientation of orbital
- **electron shell** – collection of orbitals with the same value of n
- **subshell** – orbitals that have the same n and l values
- 1) shell with principal quantum number n will consist of exactly n subshells
- 2) each subshell consists of a specific number of orbitals
  - 3) the total number of orbitals in a shell is n^2, n = principle quantum number of shell

6.6 Representation of Orbitals

6.6.1 The s Orbitals

- spherically symmetric
- **nodes** – intermediate regions where ψ^2 goes to zero
- number of nodes increases as n increases

6.6.2 The p Orbitals

- two lobes
- orbitals of a given subshell have same size and shape but differ in spacial orientation

6.6.3 The d and f Orbitals

- 5 d orbitals, 4 of which are "4 leaf clover" shaped
- one has two lobes and a "doughnut" shape in the middle
  - 7 f orbitals

6.7 Orbitals in Many-Electron Atoms

6.7.1 Effective Nuclear Charge

- effective nuclear charge – net positive charge attracting the electron
- $Z_{eff} = Z - S$ (Z_{eff} = effective nuclear charge, Z = number of protons, S = average number of electrons
- Screening effect – inner electrons shield outer electrons from full charge of nucleus

6.7.2 Energies of Orbitals

- In a many-electron atom, for a given value of n, Z_{eff} decreases with increasing value of l
- in a many-electron atom, for a given value of n, the energy of an orbital increases with increasing value of l
- **degenerate** – orbitals with the same energy

6.7.3 Electron Spin and the Pauli Exclusion Principle

- George Uhlenbeck and Samuel Boudsmit – proposed the electron spin
- Electron spin quantum number, m_s – can only have values of +0.5 and –0.5
- Pauli exclusion principle – no two electrons in an atom can have the same set of four quantum numbers n, l, m_1, and m_s
- An orbital can hold a maximum of two electrons, and they must have opposite spins

6.8 Electron Configuration

- **electron configuration –** the way electrons are distributed in orbitals
- **orbital diagram –** a box with each electron represented by a half arrow (arrow pointing=electron with positive spin, arrow pointing down=electron with negative spin)

6.8.1 Periods 1,2, and 3

- **Hund's rule** – for degenerate orbitals, the lowest energy is attained when the number of electrons with the same spin is maximized
- **Valence electrons –** outer shell electrons
- **Core electrons** – electrons in the inner shells

6.8.2 Period 4 and Beyond

- **transition elements or transition metals** – 4^{th} row of the periodic table
- **lanthanide elements** - elements 58-71 (rare-earth)
- **actinide elements –** last row of periodic table

6.9 Electron Configurations and the Periodic Table

- the periodic table is your best guide to the order in which orbitals are filled
- chromium is $[Ar]4s^1 3d^5$ rather than $[Ar]4s^2 3d^4$
- copper $[Ar]4s^1 3d^{10}$ rather than $[Ar]4s^2 3d^9$