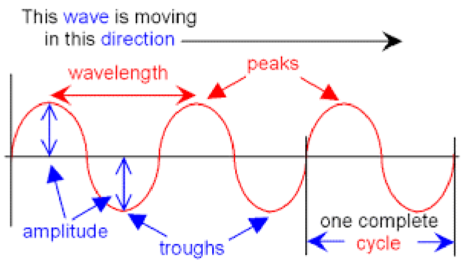
Atomic Structure

Chemistry 30 AP – Ms. Hayduk

Electromagnetic Radiation

- Energy travels through space by electromagnetic radiation
  - e.g. x-rays, microwaves, radiant heat
- Has wave-like properties and particle-like properties
- All travels at the speed of light, 2.998×10^8 m/s

Waves Characteristics



Wave Characteristics

- **Wavelength** (λ, lambda): distance between two consecutive peaks or troughs on a wave (m)
- **Frequency** (v): number of wave cycles past a certain point per unit time (Hz, Hertz or cycles/s)

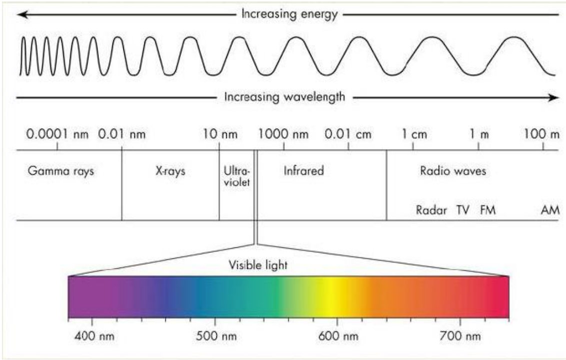
Wave Nature of Light

- Frequency and wavelength are inversely proportional
- Since speed of light is constant, as frequency increases, wavelength decreases

$$c = \lambda \nu$$

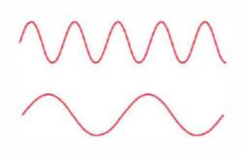
- Higher frequency also means more energy

Electromagnetic Radiation



Example 1: Light as a Wave

- Which wave below has a higher frequency?
- If one wave represents visible light, and the other represents infrared radiation, which is which?
- Which has a higher energy?



Example 2: Light as a Wave

- The yellow light given off by sodium vapour lamps, used for public lighting, has a wavelength of 589 nm. What is the frequency of this radiation?

Particle Nature of Light

- Phenomena unexplained by wave behaviour:
  1. Emission of light from hot objects (*blackbody radiation*)
  2. Emission of electrons from metal surfaces struck by light (*photoelectric effect*)
  3. Emission of light from electronically excited gas atoms (*emission spectra*)

Blackbody Radiation

- When solid objects are heated (e.g. electric stove burner, incandescent light bulb), they emit radiation
- Wavelength (colour) depends on temperature of object (kinetic energy)
- Energy released/absorbed can only be done in specific quantities (whole number multiples), called quanta

Planck's Constant

$$\Delta E = nh\nu$$

Where:

ΔE is the energy change in a system in J, Joules

n is an integer (1, 2, 3…)

h is Planck's constant, 6.626×10^{-34} J·s

ν is the frequency in Hz, or 1/s

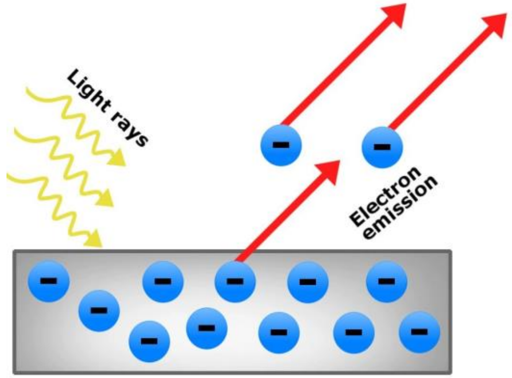
Analogy of Quantized Energy

- Potential energy walking up stairs
- Your energy increases discretely as you climb a staircase – can only step on individual stairs, not between

Example: Planck's Constant

Determine the quantum (increment of energy) that can be emit by red light with a wavelength of 7.50×10^2 nm.

Photoelectric Effect



Photoelectric Effect

- Light strikes the surface of some metals, causing an electron to be ejected
- Light must have sufficient energy to eject an electron (short wavelength)
- Energy hitting the surface behaves like a particle, or energy packet, called a **photon**
- Energy of one photon is given by:

$$E = h\nu = \frac{hc}{\lambda}$$

Example: Energy of a Photon

Calculate the energy of one photon of yellow light with a wavelength of 589 nm.

Mass of Photons

- For an object not travelling at the speed of light, De Broglie suggested:

$$m = \frac{h}{\lambda \mathrm{v}}$$

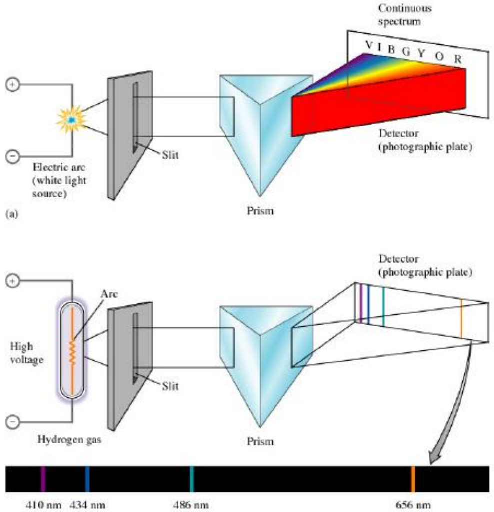
- For a photon, v is the speed of light.

Example: Wavelength

Compare the wavelength for an electron (mass = 9.11×10^{-31} kg) travelling at a speed of 1.0×10^{7} m/s with that for a ball (mass = 0.10 kg) travelling at 35 m/s.

Wavelength of Matter

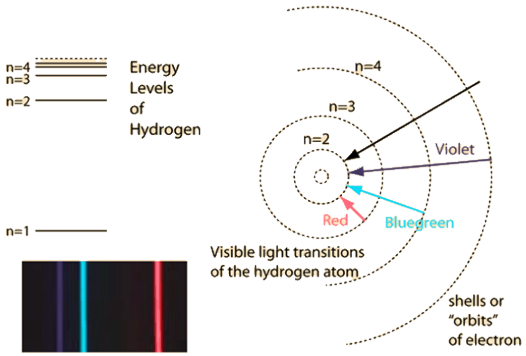
- Massive objects have smaller wavelengths and vice versa
- A beam of electrons can be diffracted like light waves
- This means any moving particle has an associated wavelength
- **All matter has particulate and wave properties**



Bohr Model for Hydrogen

- Single electron – limited to certain energy values (n = 1, 2, 3…)
  - n is the **principal quantum number**
- Most stable state = ground state (n = 1)
- Energy (photons) supplied to atom moves electron to higher energy level = excited state
- Excited electron releases photon when it drops back down to ground state

Bohr Model for Hydrogen



Bohr Model + Line Spectra

- Line spectra is formed from the movement of electrons between quantized energy states
- If an electron moves from higher to lower E states, photon is emitted and emission line is observed

Bohr Equation

Calculate energy required to move an electron from one energy state to another, or to remove it completely, for **hydrogen**:

$$\Delta E = -2.178 \times 10^{-18}\left(\frac{1}{n_{final}^2} - \frac{1}{n_{initial}^2}\right)$$

Example 1: Bohr Equation

For an electron in an hydrogen atom, calculate the energy needed to move it from n = 1 to n = 3. What is the wavelength of this light? Is it absorbed or emitted?

Example 1: Bohr Equation

For an electron in an hydrogen atom, calculate the energy needed to remove it from n = 1.

Bohr Model Limitations

- Great for explaining H, but not as good for other spectra
- Electron does not orbit the nucleus in a fixed path

Quantum Mechanical Model

- Impossible to determine electron location <u>and</u> velocity (Heisenberg Uncertainty Principle)
- Describes energy of electron precisely, but location in terms of probabilities
- Schrodinger developed wave functions – electron probability density to show where electrons would likely be found around the nucleus

Orbitals

- Electrons don't follow specific orbits
- Each Schrodinger wave function is an **orbital**, which is a specific distribution of electron density in space (probability)
- Each has characteristic energy and shape

Quantum Numbers

1. Principal quantum number, n
   - Integer values 1, 2, 3…
   - Increases for larger orbitals – electrons further from the nucleus
   - Higher energy electrons for larger n
2. Angular momentum quantum number, l
   - 0 to n-1
   - Number corresponds to a letter, which designates a shape
   - 0 = s, 1 = p, 2 = d, 3 = f

Quantum Numbers

3. Magnetic quantum number, m_l
   - Values from $-l$ to $+l$
   - Determines the orientation of the orbital

Thinking Activity!

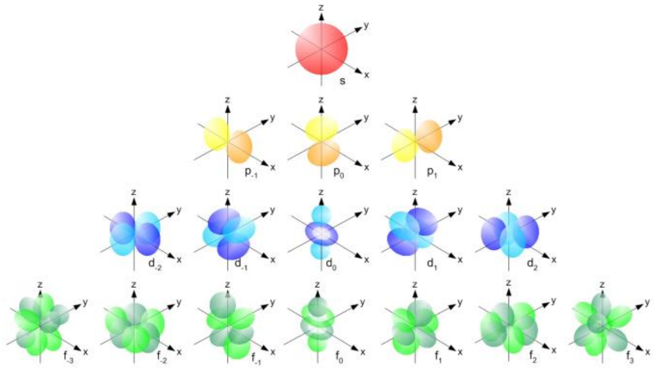
Each unique configuration of n, l and m_l corresponds to one orbital.

For each value of n from 1 to 4, determine:

- Possible values of l
- Subshell designation
- Possible values of m_l
- Number of orbitals in subshell
- Total number of orbitals in shell

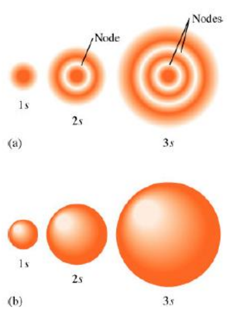
n	Possible Values of l	Subshell Designation	Possible Values of m_l	Number of Orbitals in Subshell	Total Number of Orbitals in Shell
1	0	1s	0	1	1
2					
3					
4					

Orbital Shapes



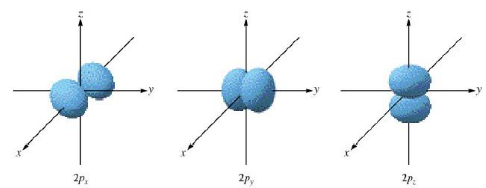
Orbital Shapes

- s – spherical, and size increases with n; no electrons at nodes



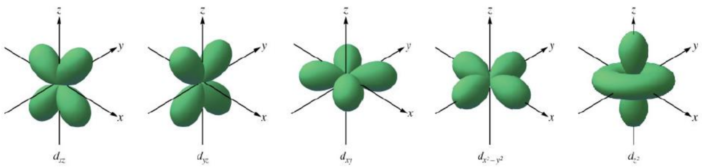
Orbital Shapes

- p – one plane that slices through nucleus and divides into two halves; no electrons on nodal plane; three orientations



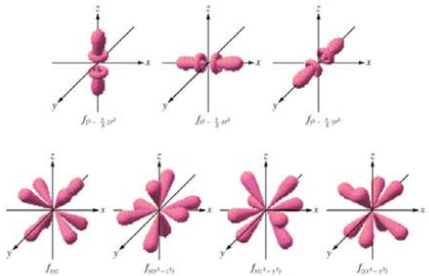
Orbital Shapes

- *d* – two planes that slice through nucleus and divides into four sections; five orientations



Orbital Shapes

- *f* – three planes that slice through nucleus and divides into eight sections; seven orientations



Electron Spin

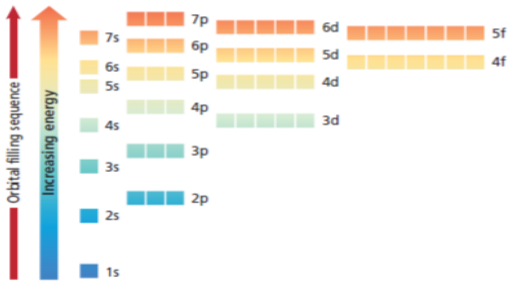
- Final quantum number, m_s, accounts for spin of electron
- Determined due to interactions of electrons with magnetic field
- Can be -1/2 or +1/2

Pauli Exclusion Principle

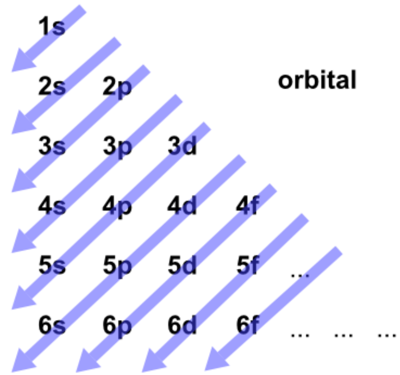
- Only two electrons can occupy any orbital
- Must have opposite spins (different m_s)

Aufbau Principle

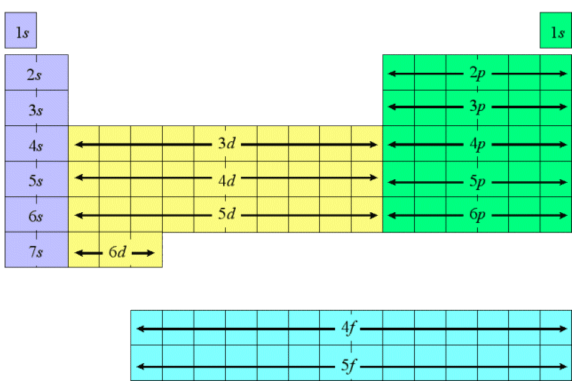
- electrons occupy the lowest energy orbitals first, one at a time



Orbitals

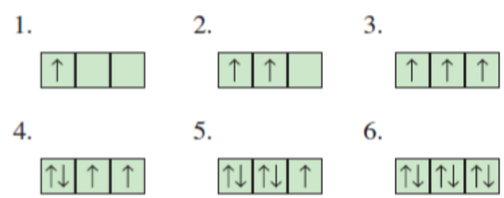


Electron Configuration



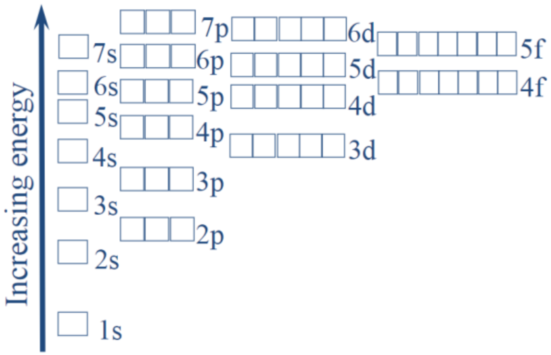
Hund's Rule

- Single electrons with same spin must occupy each equal energy orbital before a second electron can be in an orbital



Thinking Activity!

Fill this orbital diagram for calcium.



Magnetism

- Magnets have positive and negative poles – opposites attract/likes repel
- **Diamagnetic** – not magnetic, when all electrons are paired in orbitals
- **Paramagnetic** – magnetic, unpaired electrons in orbitals

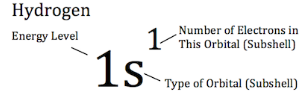
Example: Magnetism

- Is calcium diamagnetic or paramagnetic?

Electron Configuration

- Explains arrangement of atoms in orbitals when they are in lowest possible energy state (ground state)
- Can be in atoms or ions
- Written as a list of orbitals, in order (see Aufbau)

Electron Configuration of Hydrogen



Examples: Electron Configuration

H

B

Na

Cl

Ag

Sn

Noble Gas Configuration

- Write the noble gas from the period above in square brackets, then continue electron configuration from that point
- Example:

  Mg ($1s^2 2s^2 2p^6 3s^2$) becomes:

  $[Ne]3s^2$

Examples: Noble Gas Configuration

Ti

Cd

Cl

Exceptions to Aufbau

- Some elements fill or half-fill a higher energy orbital from a lower energy orbital
- Commonly, electrons will drop from an s-orbital to the d-orbital

Examples: Aufbau Exceptions

Cu

Cr

Valence and Core Electrons

- Valence electrons are those in highest energy level (*n*) – available to bond
- Core electrons are inner electrons in full, stable orbitals that are unavailable for bonding

Example: Valence Electrons

How many valence electrons does Sb have?