Chapter 4: Arrangement of Electrons in Atoms

Honors Chemistry

Section 4.1 – Atomic Models

- Dalton – indestructible mass
- Thomson – Plum Pudding Model
- Rutherford – nucleus
- Bohr – based on the solar system
- Schrodinger – mathematics based orbitals

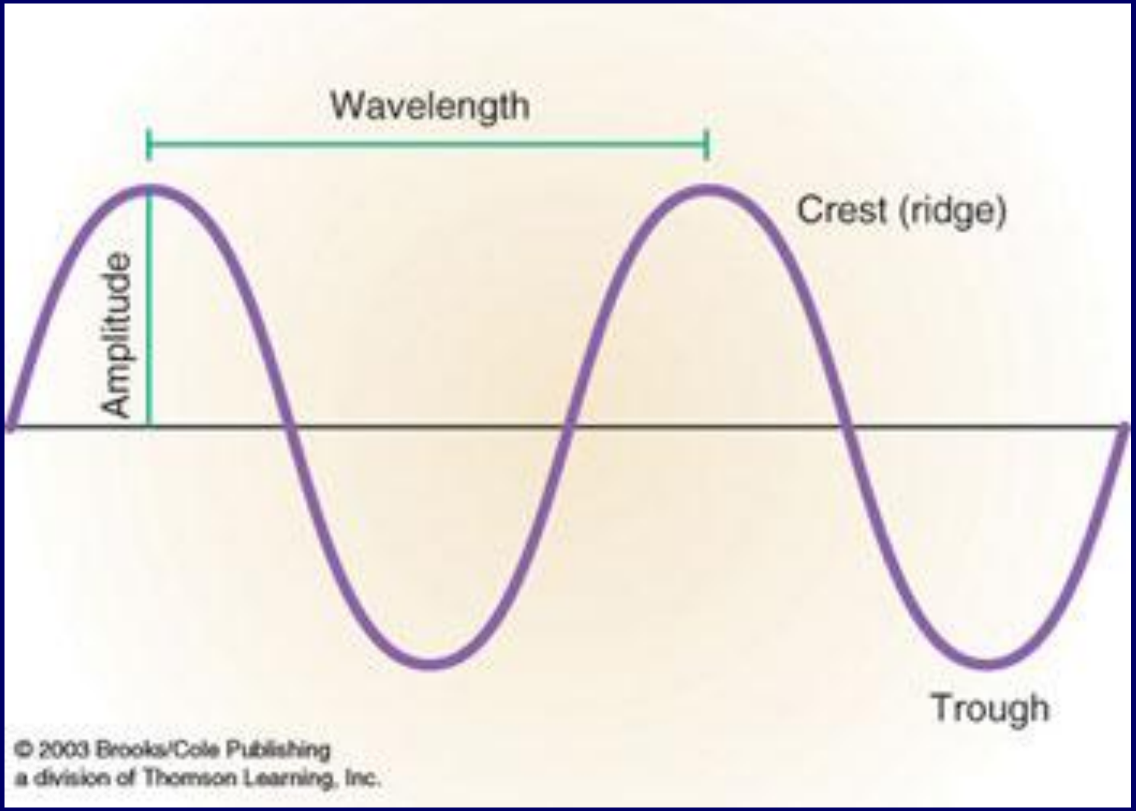
Light and Atomic Spectra

- Isaac Newton (1642-17270) thought that light consisted of particles.
- By 1900, most scientists believed that light was made up of waves.

Light & Atomic Spectra

- According to the wave model, light consists of electromagnetic waves
- The height of the wave is called the amplitude

Wave model of light



Wave Description of light

Electromagnetic radiation:

- A form of energy that exhibits wavelike behavior as it travels through space.

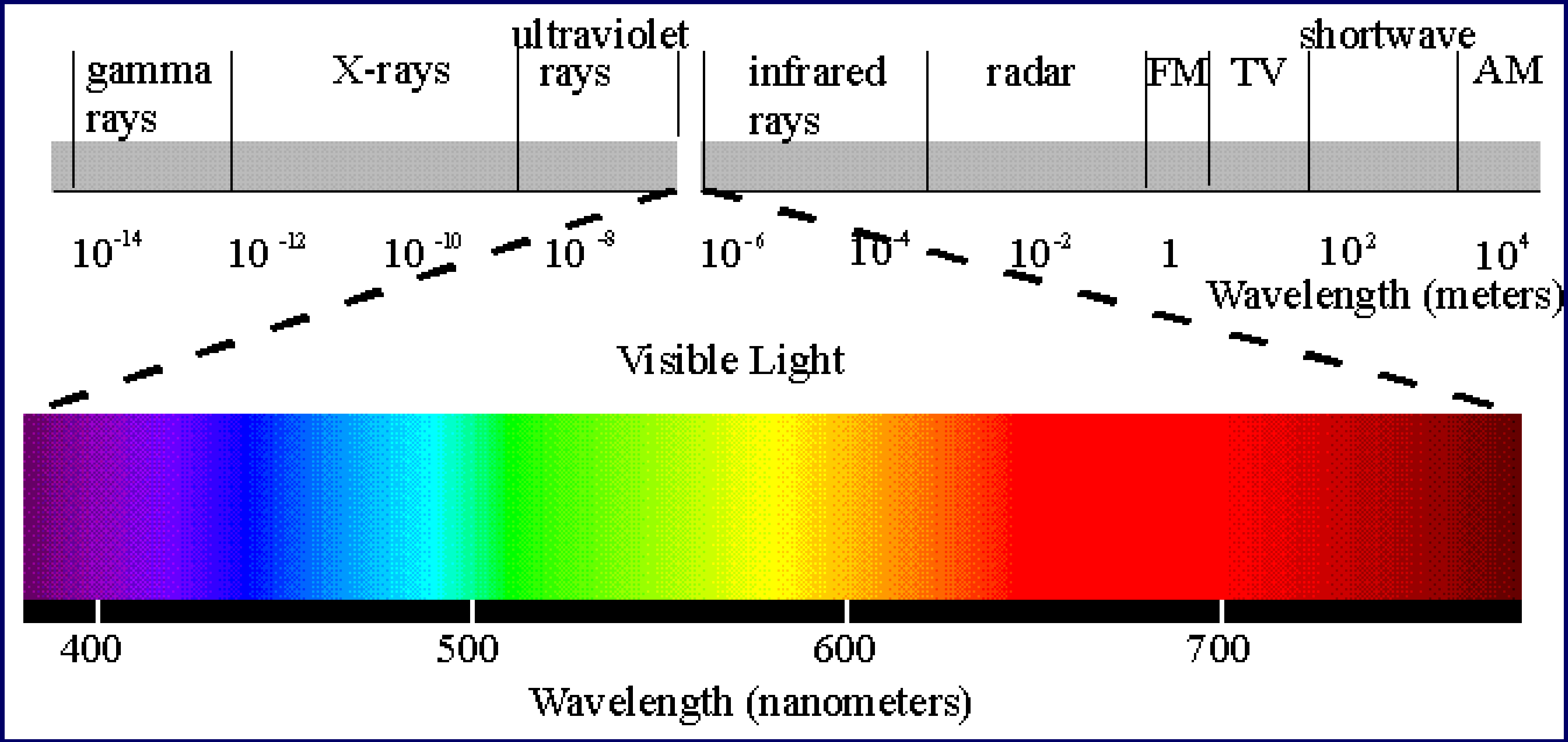
Electromagnetic spectrum:

- All the forms of electromagnetic radiation

Speed of electromagnetic radiation

- All forms of emr travel at a constant speed
- $c = 3.0 \times 10^8$ m/s

Electromagnetic spectrum



Wave model of light

$$c = \lambda \times \nu$$

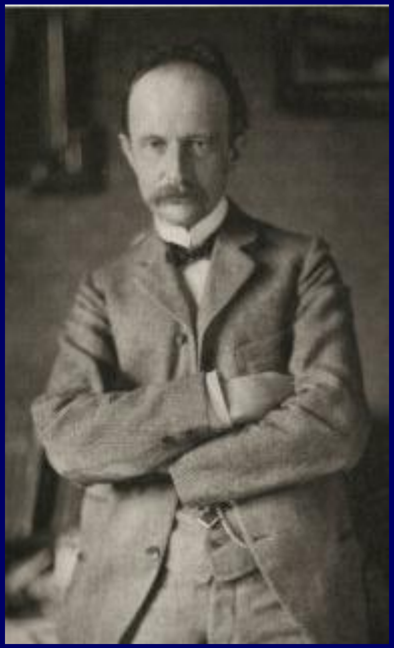
Speed	Wavelength	Frequency
m/s	m	Hz (hertz) 1/s

c = Speed of light = 3.00×10^8 m/s

Photoelectric Effect

- The photoelectric effect refers to the emission of electrons from a metal when light shines on the metal
- It takes a specific frequency of light to make a certain metal eject a photoelectron
- The wave model predicts that light of any frequency should cause emission of an electron

The Particle Description of Light



In 1900 Max Planck proposed that objects emit energy in small discrete packets that he called *quanta*

- A *quantum* of energy is the minimum quantity of energy that can be lost or gained by an atom.

He proposed the relationship:

$$E = h\,\nu$$

Energy of Photons

The energy of an individual photon is directly proportional to its frequency.

$$E = h \times \nu$$

Energy = Plank's constant x frequency

Photons with greater frequency (shorter wavelengths) have greater energy.

Particle Wave Duality

In 1905 Albert Einstein expanded Planck's theory by introducing the idea that electromagnetic radiation has a dual wave-particle nature.

Light can be considered to considered as a stream of particles, called *photons*.

- A *photon* is a particle of electromagnetic radiation having zero mass and carrying a quantum of energy.

Photoelectric Effect

Einstein explained the photoelectric effect:

- Electromagnetic radiation is absorbed by matter only in whole numbers of photons
- In order for an electron to be ejected from a metal surface, the electron must be struck by a photon possessing at least the minimum energy required to knock it loose.

$$E_{photon} = h \times \nu$$

Calculating Frequency

What is the frequency of light with a wavelength of 500 nm?

$c = \lambda \times \nu$

$\lambda = 500$ nm $= 5 \times 10^{-7}$ m

$c = 3.00 \times 10^{8}$ m/s

3.00×10^{8} m/s $= (5 \times 10^{-7}$ m$)\ \nu$

$\nu = 6.00 \times 10^{14}$ Hz

Calculating Energy

Determine the energy of light with a frequency $\nu = 6.00 \times 10^{14}\ s^{-1}$.

$E = h \times \nu$

$\nu = 6.00 \times 10^{14}\ s^{-1}$

$h = 6.63 \times 10^{-34}\ J \bullet s$

$E = (6.63 \times 10^{-34}\ J \bullet s) \times (6.00 \times 10^{14}\ s^{-1})$

$E = 3.98 \times 10^{-19}\ J$

Line Emission Spectrum: Hydrogen

- When electric current is passed through a vacuum tube containing hydrogen gas, a pink glow is observed
- If the light is passed through a prism it is separated into four bands of lines of visible light
- The four bands are part of hydrogen's emission line spectrum
- Two additional series were discovered

The Hydrogen Spectrum

There are three groups of lines in the hydrogen spectrum

- Only one group, the Balmer series, is visible
- Lyman series = UV
- Paschen series = IR

Emission Spectrum

- The lowest energy state of an atom is called the *ground state*.
- A state in which an atom has a higher potential energy than it has in its ground state is called an *excited state*.
- (Think of Ms. Agostine with too much coffee)

Emission Spectrum

Classical atomic theories predicted that hydrogen would emit a continuous range of frequencies, a *continuous spectrum.*

Attempts to explain hydrogen's line emission spectrum lead to a new theory called *quantum theory.*

When an excited hydrogen atom falls to its ground state it emits a photon of radiation

The Hydrogen Spectrum

- It absorbs a specific amount of energy, and emits that same amount
- The energy is emitted when the e^- falls back to ground state (emission of light)

Bohr's Model

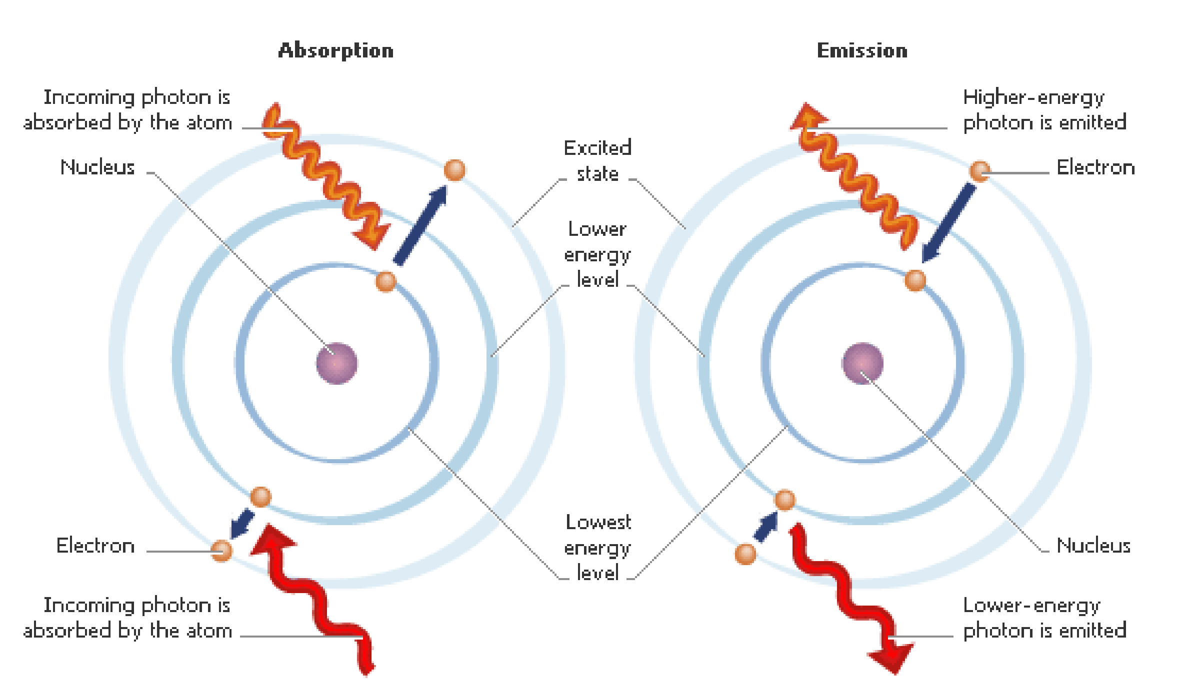
- Bohr – proposed that electrons have a fixed energy and move in energy levels around the nucleus – which is why they don't fall into the nucleus

Bohr’s Model

- The energy levels are like the rungs of a ladder – electrons cannot be in between levels, and need a specific amount of energy to move from one to another
- Bohr’s model of the hydrogen atom explained the observed spectral lines.
- The Bohr model did not explain the spectra of atoms with more than one electron.

How Atoms produce light

- Atoms absorb and release photons as electrons move from one energy level to another



Section 4.2 The Quantum Model

Electrons as Waves

In 1924 Louis DeBroglie suggested that electrons be considered as waves confined around an atomic nucleus.

Electrons as waves

The electron waves could only exist at specific frequencies that correspond to specific energies- the quantized energies associated with the Bohr orbits.

His hypothesis was confirmed by experiments

Heisenberg Uncertainty Principle

In 1927 Werner Heisenberg proposed his uncertainty principle:

- It is impossible to know simultaneously both the position and the velocity of an electron or any other particle

Simply stated:

- You cannot tell where (position) an e^- is and how fast (velocity) it is going at the same time

Schrodinger Wave Equation

- In 1926 Erwin Schrodinger developed an equation that treated electrons in atoms as waves.
- Together with the Heisenberg uncertainty principle it laid the foundation of modern quantum theory.

Quantum Theory

- Describes mathematically the wave properties of electrons and other very small particles.
- Scientists use Quantum numbers to describe the probability of finding an electron in an atom

Quantum Mechanical Model

- Based on Schrodinger's equation
- The energy levels are not equally spaced like a ladder – they get closer the farther from the nucleus you go
- The higher the e^-, the easier it leaves the atom

Quantum Mechanical Model

- There is no exact path for e^- to take
- Instead, there are areas of high probability to find an e^-, and areas with a low probability to find an e^-

Quantum Mechanical Model

- The probability of finding an e^- is represented by a fuzzy cloud
- The cloud shows where the electron is ~90 % of the time

Principle Quantum Number

The principle (main) energy levels are assigned numbers according to their energy

n = 1, 2, 3, 4, etc

1 has lowest energy

Angular Momentum Quantum Number (l)

Indicates the shape of the orbital: each principle energy level has 1 or more sublevels

(The number of sublevels = the energy level #)

- First level (1) has 1 sublevel called the 1s
- Second level (2) has 2 sublevels called 2s & 2p
- Third level (3) has 3 sublevels called 3s, 3p, and 3d
- Fourth level (4) has 4 sublevels called 4s, 4p, 4d, and 4f

Magnetic Quantum Number (m)

Indicates the orientation of an orbital around the nucleus.

Values of m are whole numbers, including zero, from $-l$ to $+l$

- Each s sublevel has only one orbital
- Each p sublevel has 3 orbitals: x, y and z
- Each d sublevel has 5 orbitals
- Each f sublevel has 7 orbitals

Atomic Orbitals

Energy Level	**# of Sublevels**							
n=1	1	s						
n=2	2	s	p					
n=3	3	s	p	d				
n=4	4	s	p	d	f			
n=5	5	s	p	d	f	g		
n=6	6	s	p	d	f	g	h	
n=7	7	s	p	d	f	g	h	i

[Atomic Orbital Visualizations]

Atomic Orbital Pictures

http://winter.group.shef.ac.uk/orbitron/AOs/2s/index.html

http://www.uwosh.edu/faculty_staff/gutow/Orbitals/Cl/Cl_AOs.shtml

Spin Quantum Number

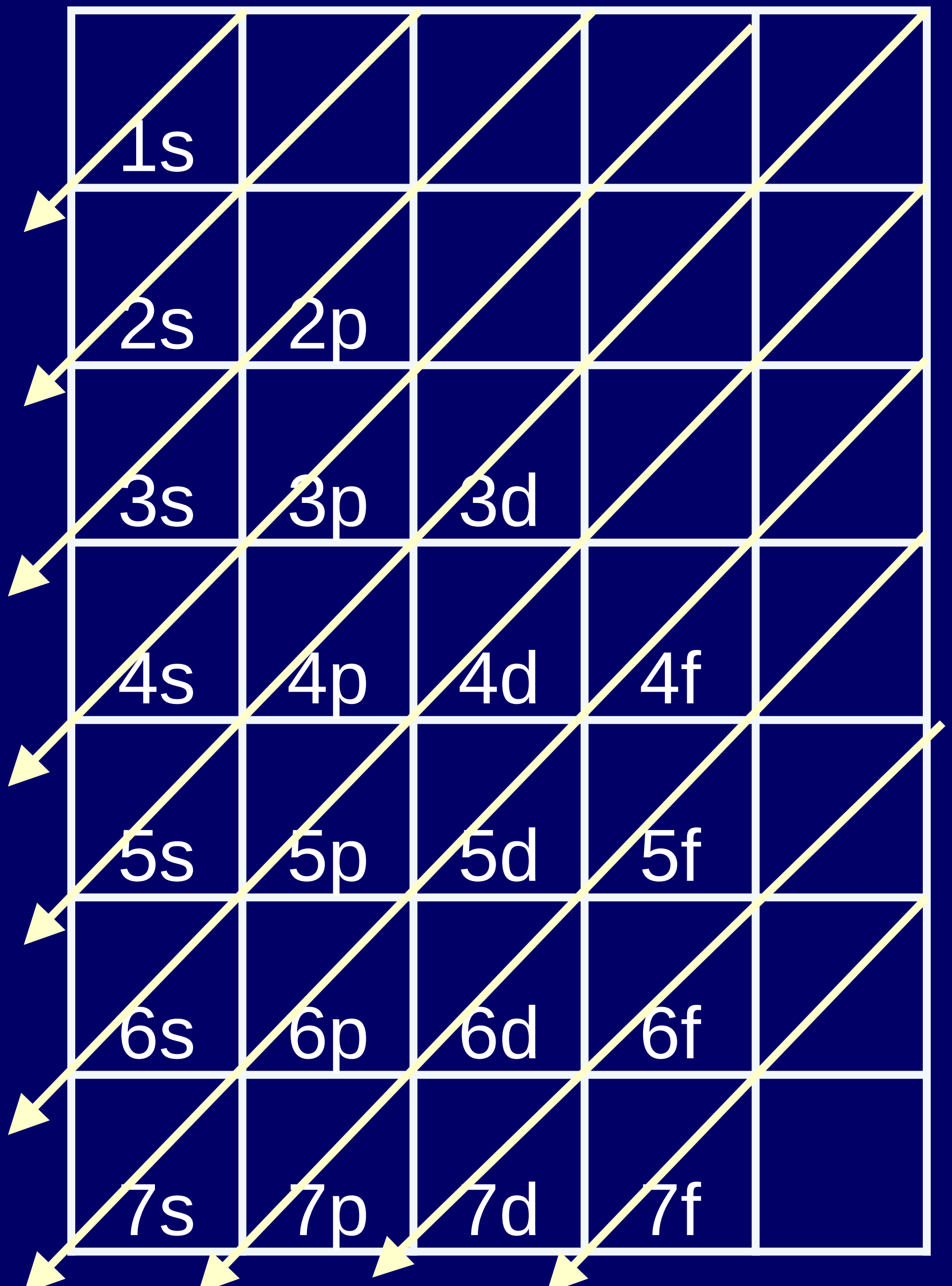
- The spin quantum number has two possible values: = +½ and – ½
- Each orbital may only contain a maximum of 2 electrons
  - n = 1 has only 1 sublevel, “s”
  - The maximum number of electrons for this level is therefore 2

Atomic Orbitals

Energy Level	# of Sublevels					Total # of Electrons
n=1	1	s				2
n=2	2	s	p			8
n=3	3	s	p	d		18
n=4	4	s	p	d	f	32

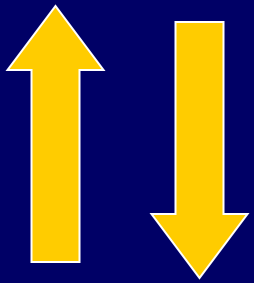
Electrons in orbitals

- **Aufbau Principle**: states that electrons (e^-) enter the lowest energy orbitals first
- The next slide shows the order in which orbitals fill
- The *Aufbau principle* (from the German Aufbau meaning "building up, construction)


1s
2s
2p
3s
3p
3d
4s
4p
4d
4f
5s
5p
5d
5f
6s
6p
6d
6f
7s
7p
7d
7f

Electrons in orbitals

- **Pauli Exclusion Principle**: states an orbital can hold a maximum of 2 electrons
- They must have opposite "spins"



Electrons in orbitals

- **Hund's Rule**: States that when orbitals have equal energy, one e^- goes into each orbital before any are filled – each would have 1 e^- with parallel spins

Electron Configuration

- 3 rules
  - Aufbau, Pauli-Exclusion, & Hund’s
- Draw orbitals according to the 3 rules↥
- Exceptions to the rules!
  - Especially: Cr, Cu, & Mo

Exceptions to Aufbau Rule:

- ^{24}Cr, the aufbau principle predicts the an electron configuration of [Ar]$3d^4 4s^2$ but experimentally we find it to be [Ar]$3d^5 4s^1$
- ^{29}Cu, the predicted electron configuration is [Ar]$3d^9 4s^2$ but experimentally we find it to be [Ar]$3d^{10} 4s^1$
- ^{42}Mo, the predicted electron configuration is [Kr]$4d^4 5s^2$ but experimentally we find it to be [Kr]$4d^5 5s^1$

Electron Configuration

Three ways to represent configurations:

- Orbital Notation
- Electron Configuration Notation
- Noble Gas Notation