Atomic Theory

At the particulate (atomic) level:
Arrangement & energies of electrons define chemical properties
(Basis of the Periodic Table)

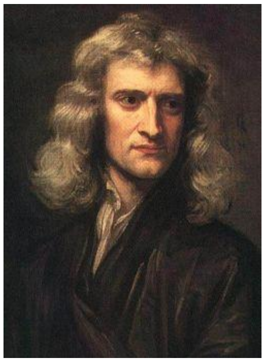
Electrons are responsible for observed chemical reactions
(Nucleus is NOT involved in ordinary chemical reactions)

Arrangement & energies of electrons predict chemical behavior

Based on Quantum (Discrete Energy) Mechanics
Particles behave as particle-waves (a duality)
Particle-wave location only a probability function

Quantum Theory emerged after 300 year debate

Light
Wave or
Particle?



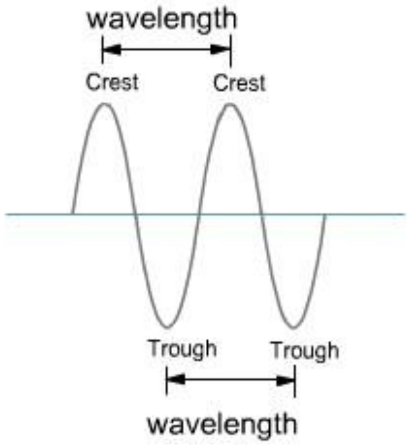
Christian Huygens

Issac Newton

Particles vs. Waves

Particles = like tiny BB's
Wave = repeating oscillation
Wavelength (l) = distance between adjacent identical points
Frequency (n) = # of waves passing a fixed point in one second

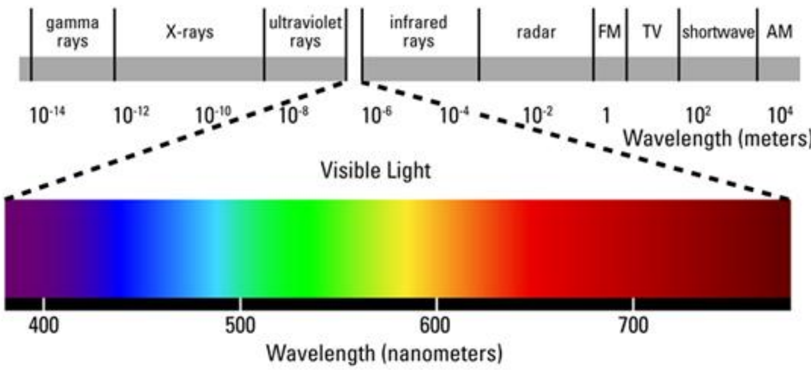
Frequency & Wavelength are inversely related:
high frequency means short wavelength
low frequency means long wavelength



c = speed of light (in vacuum)
= 299,792,458 m/sec
(3×10^8 m/sec)
= 186,000 mi/sec

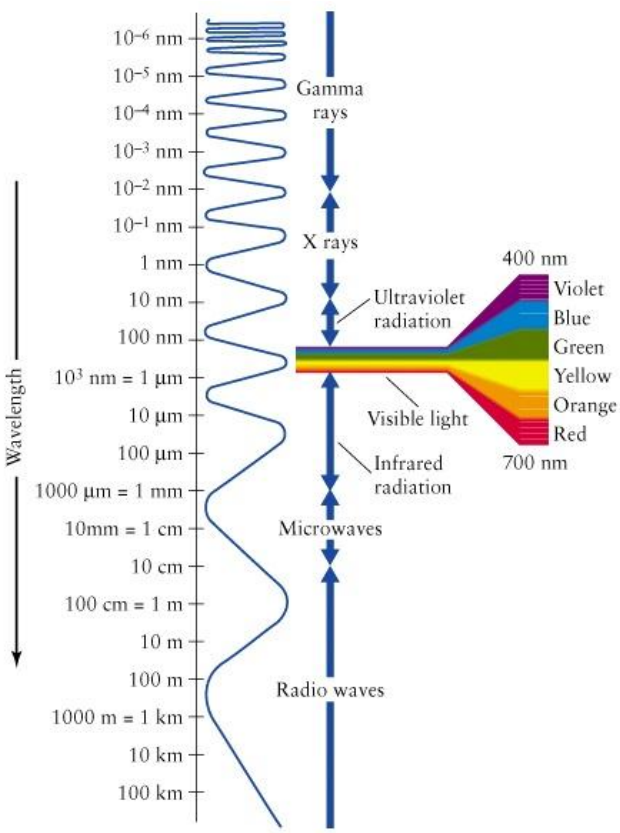
c from Latin *celeritus* "swiftness"

Electromagnetic Spectrum



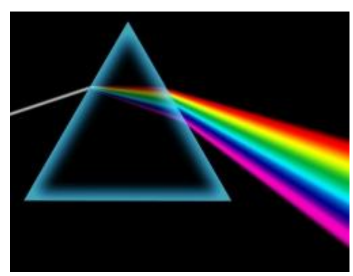
Wave energy & frequency are directly related.
frequency increases, energy increases
energy decreases, frequency decreases

Wave energy & wavelength are inversely related
wavelength increases, energy decreases
wavelength decreases, energy increases



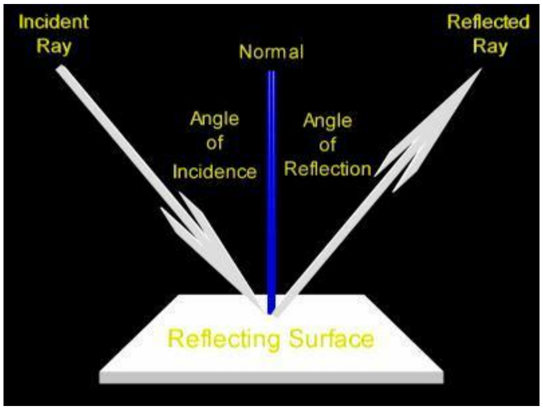
Light

Only a small portion
Of
Electro-magnetic spectrum



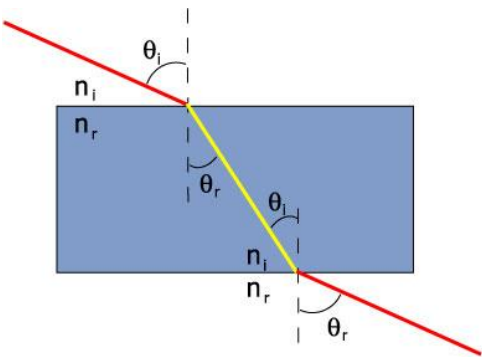
Properties of Light

Reflection



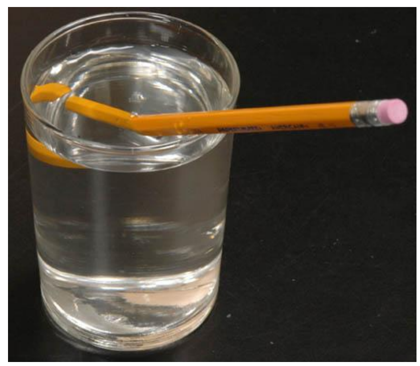
Mirror

Refraction

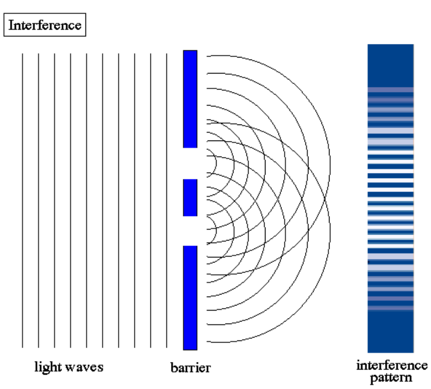


Bending

Lenses



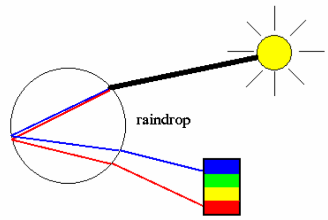
Interference

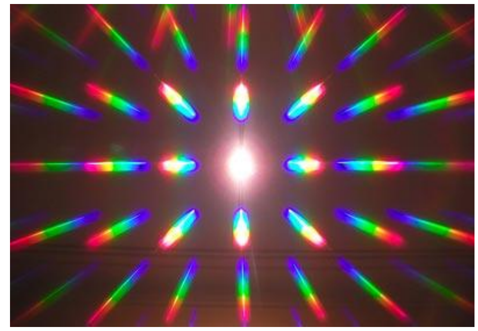


Amplification
Cancellation

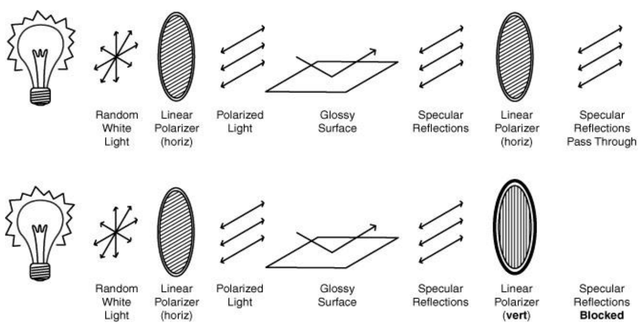
Diffraction

Prisms
Rainbows

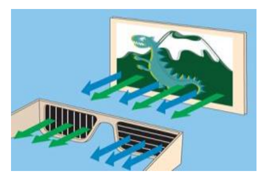




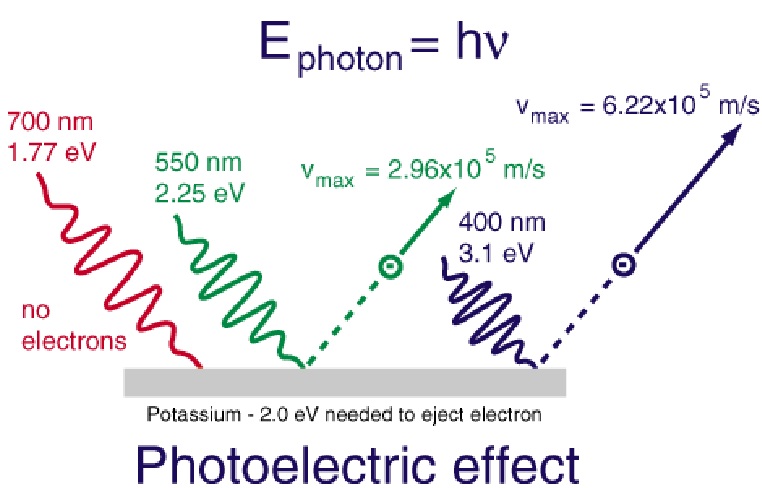
Polarization



Glare Filters
3-D Visualizations
Strain Visualizations



Photoelectric Effect – light creates current (electrons) flow



Not all colors (energies)
Create photoelectric effect

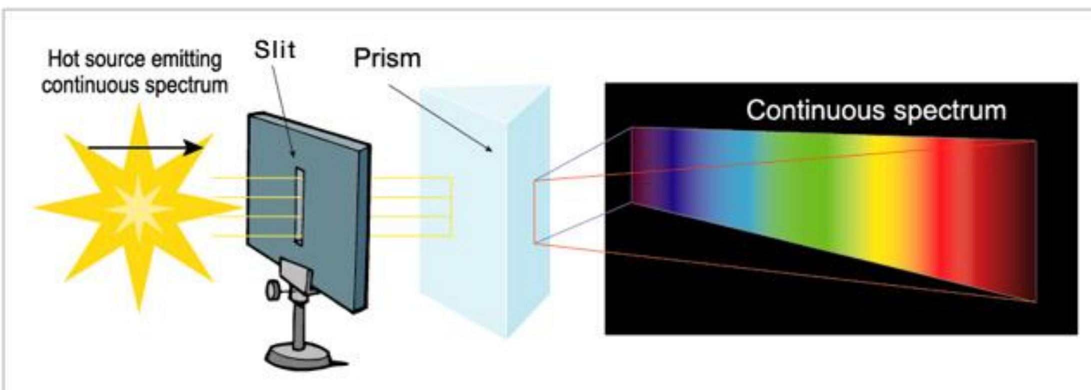
Only Possible by
Energy transfer of particles

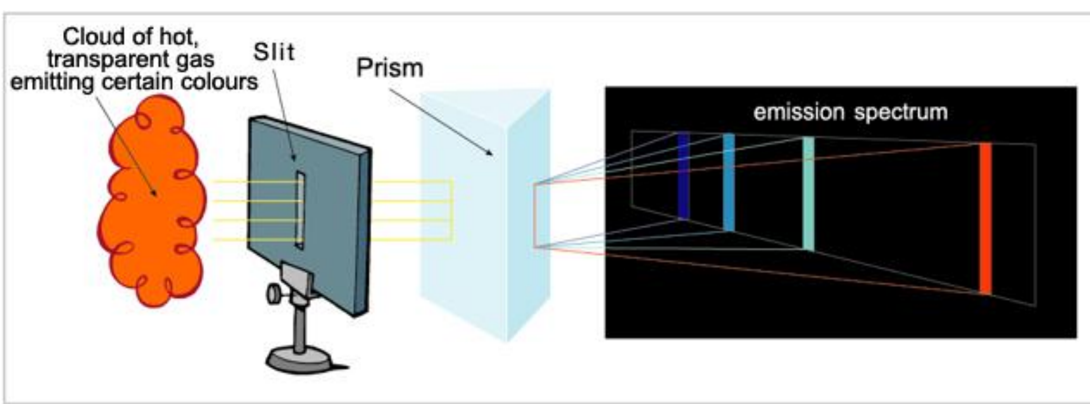
Einstein – Nobel Prize

Summary

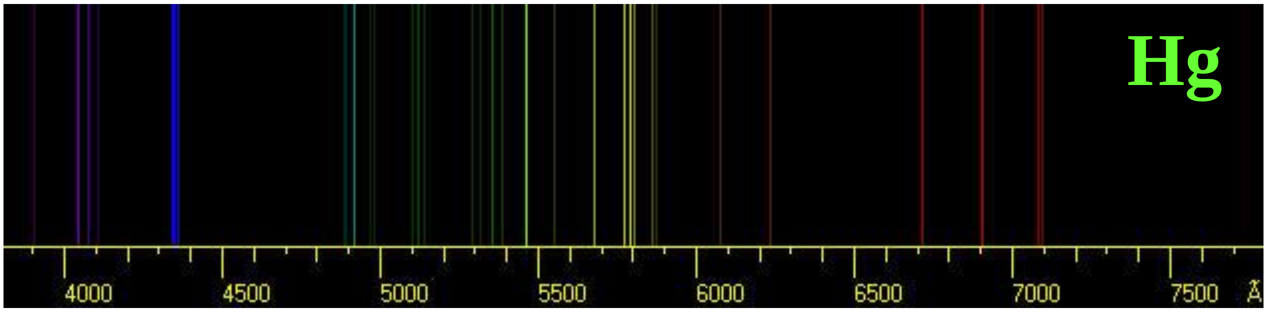
Phenomenon	Can be explained in terms of waves.	Can be explained in terms of particles.
Reflection	✓	✓
Refraction	✓	✓
Interference	✓	⊗
Diffraction	✓	⊗
Polarization	✓	⊗
Photoelectric effect	⊗	✓

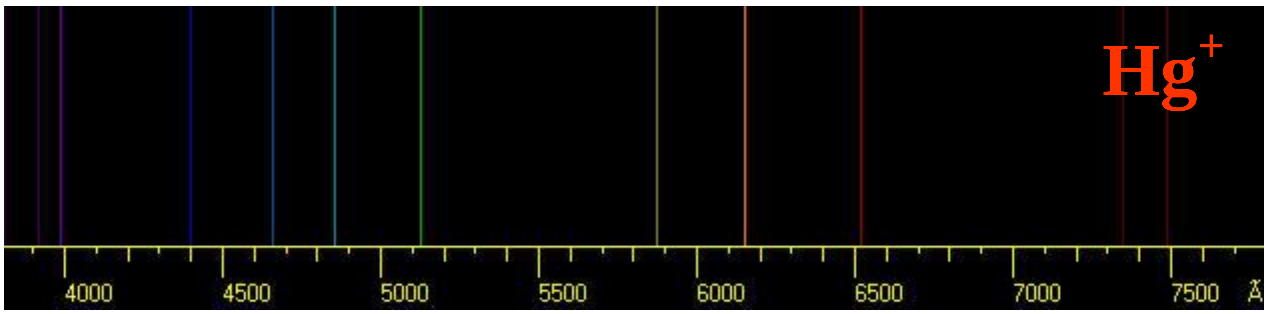
Spectrum Experiment

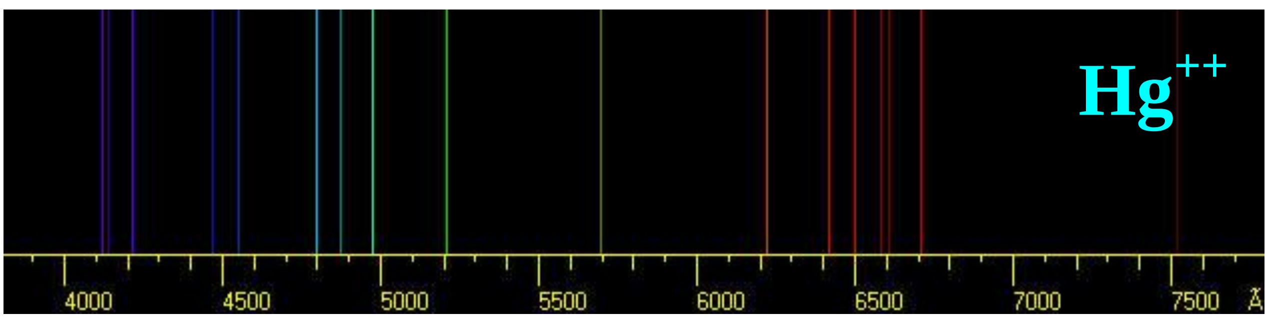




Emission Spectra: Measure of electron energy

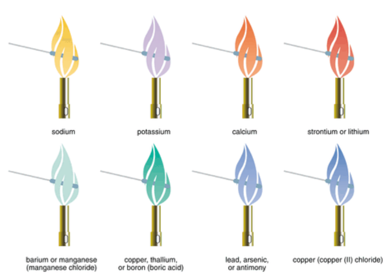


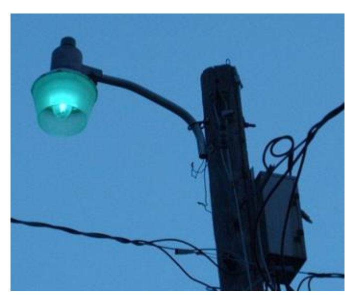




Emission Spectra

Determines Observed Colors Of lights & flames



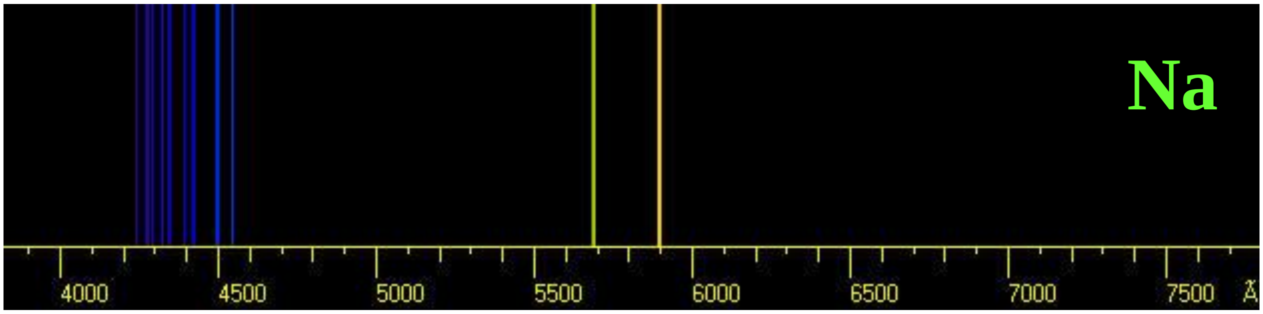


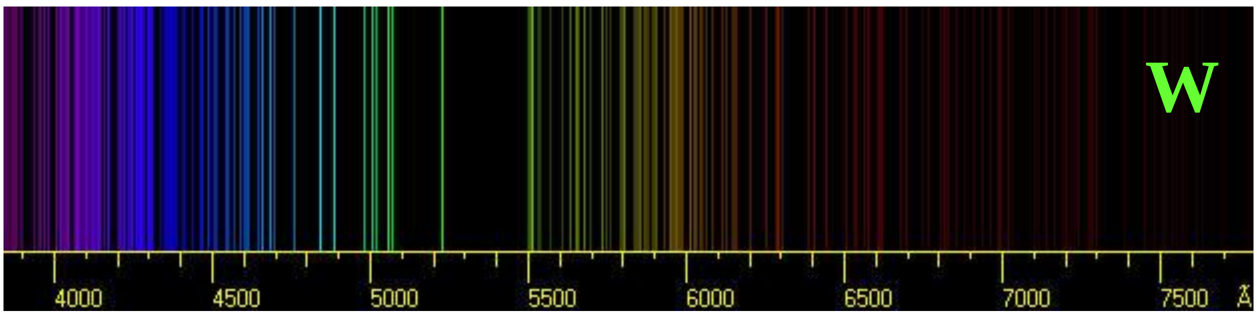
Na Vapor

"Fireplace Crystals"

Hg Vapor

Emission Spectra: Indicators of Electron Energy



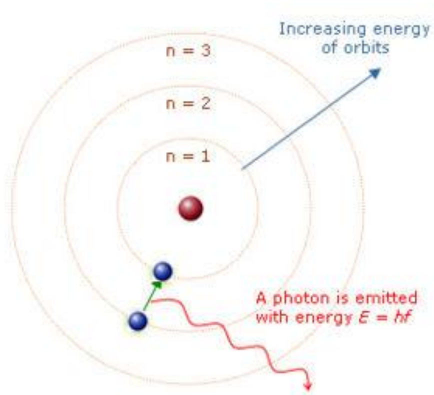


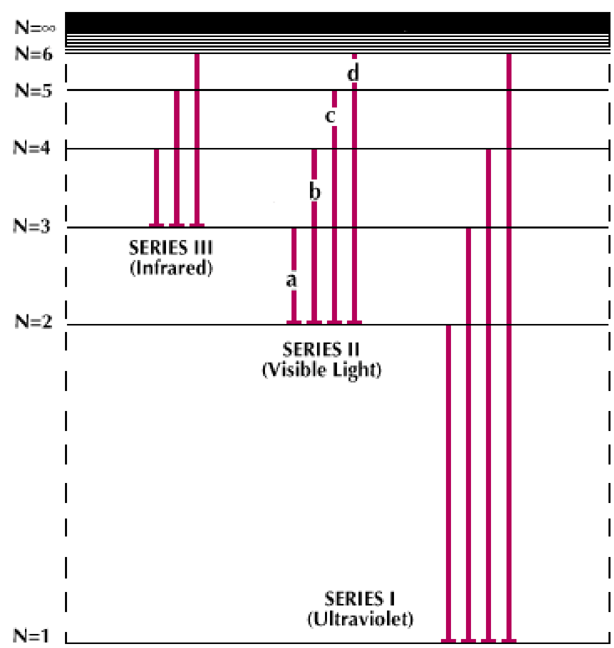
Emission spectra – Discrete energy lines   **Define electron energies**

Different electron energies

Define chemical properties
Define Periodic Table Arrangement

Electron States





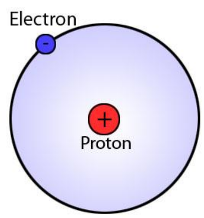
Ground State ➔ Absorbs energy ➔ Excited state
Excited State ➔ Releases Energy ➔ Ground State

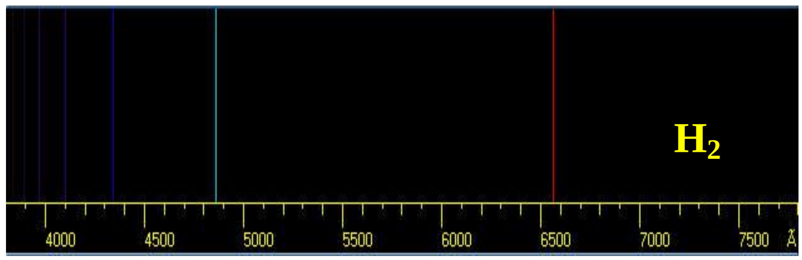
Emission Spectra: Excited State ➔Ground State
Absorption Spectra: Ground State ➔ Excited State

Bohr Model of the Hydrogen Atom

Energies of electrons are quantized
Electrons (particles) reside in specific orbits around the nucleus
Behavior explained by Coulomb's law of magnetic attraction
Only worked for hydrogen atom with one electron

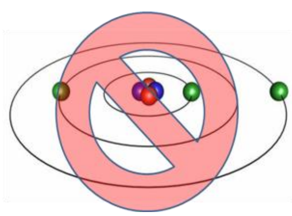
A stepping-stone to quantum theory



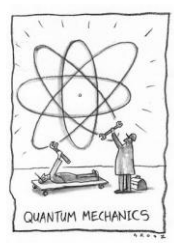


Heisenberg Uncertainty Principle
Based on a wave-particle duality

It is not possible to simultaneously know electron position & velocity
It is not possible to know the exact path of electron travel (orbits)



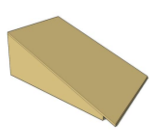
Modern Atomic Theory



Wave-Particle Duality

Explaining light and sub-atomic particles requires duality

Quantum Mechanics
Discrete, non-continuous values of energy



Stair = discrete steps ➔ Quantized Process
Ramp = Continuous Process

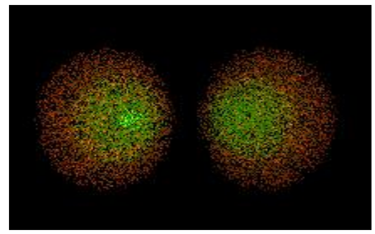
Schrodinger (1925) Wave Equation

H Ψ = E Ψ

There exists a wave function, H, that describes the energy, E, of wave system Ψ

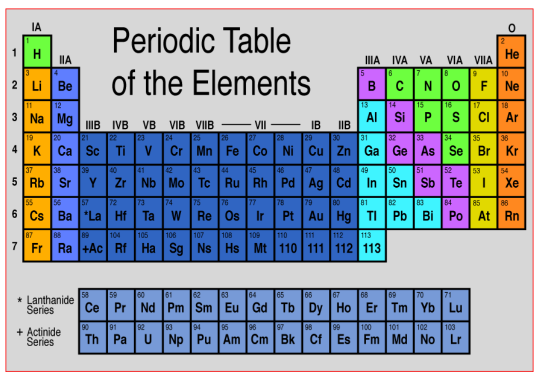
In this construct for electrons, Ψ^2 = probability of finding an electron in space

$$\psi_{3,1,-1} = \frac{2}{27\sqrt{\pi r_0^5}} \sin\vartheta \cdot r \cdot \left(1 - \frac{r}{6r_0}\right) \exp\left(-r/3r_0\right) \cdot e^{-i\varphi}$$



Defines all possible electron configurations in terms of 4 quantum numbers
(analogous to an indexing or addressing system)

The Periodic Table can be explained using these numbers



Quantum Numbers

Name	Symbol	Meaning
Principal	n	Shell
Azimuthal	l	Sub-shell Type
Magnetic	m_l	Sub-Shell Orientation
Spin	m_s	Spin

Principle Quantum Number

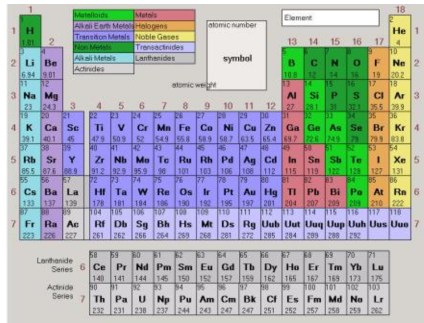
Value of 1, 2, 3, … infinity

Represents principle energy (shell) of an electron
Increasing n ➔ increasing energy
Increasing n ➔ increasing distance from the nucleus

Corresponds to the n value (row) on the periodic table

n

Integer
Along left of table

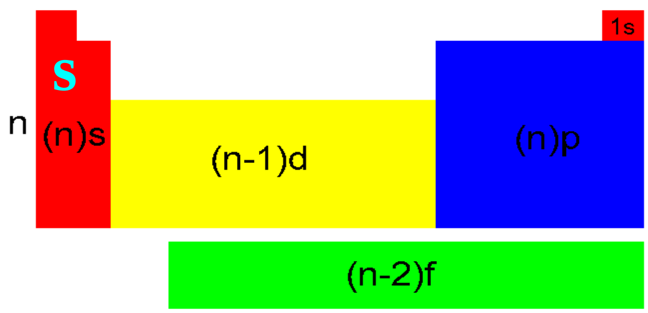


Azimuthal Quantum Number

value of $0 \leq l \leq n-1$
Represents orbital type

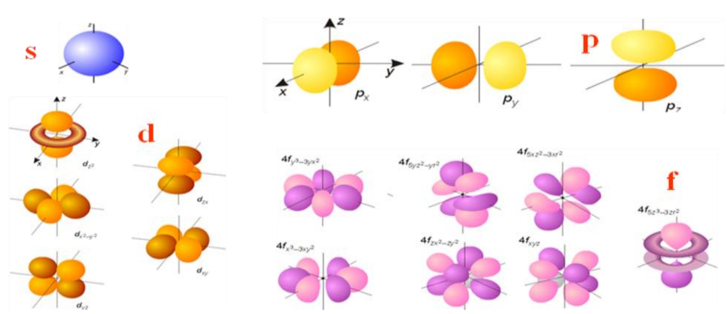
- $l = 0$ ➔ s orbital (spherical)
- $l = 1$ ➔ p orbital (dumb-bell)
- $l = 2$ ➔ d orbital (varied shape)
- $l = 3$ ➔ f orbital (varied shape)

Corresponds to "Orbital Blocks" in the periodic table



Magnetic Quantum Number (m_l)

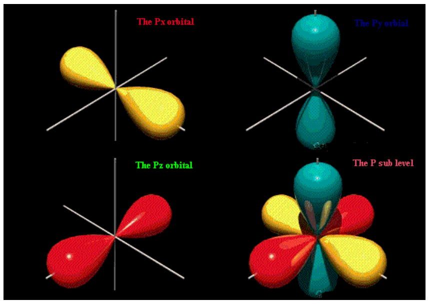
Value of $-l \leq m_l \leq l$
Represents spatial orientation (with respect to external field)
Each orbital has a separate (magnetic) quantum number



Planets Travel in Orbits; Electrons Occupy Orbitals

Pauli-Exclusion Principle

Maximum 2 electrons per orbital (orbital may have 0, 1 or 2 electrons)
No two electrons have same set of quantum numbers



For p orbitals:

3 orbitals/shell x 2 electrons/orbital =
6 maximum p orbital electrons /shell

Spin Quantum Number (m_s)

Value of either + ½ or – ½ (for maximum 2 electrons / orbital)
NOT spin around axis (electron a particle-wave, not particle)

Hund's Rule

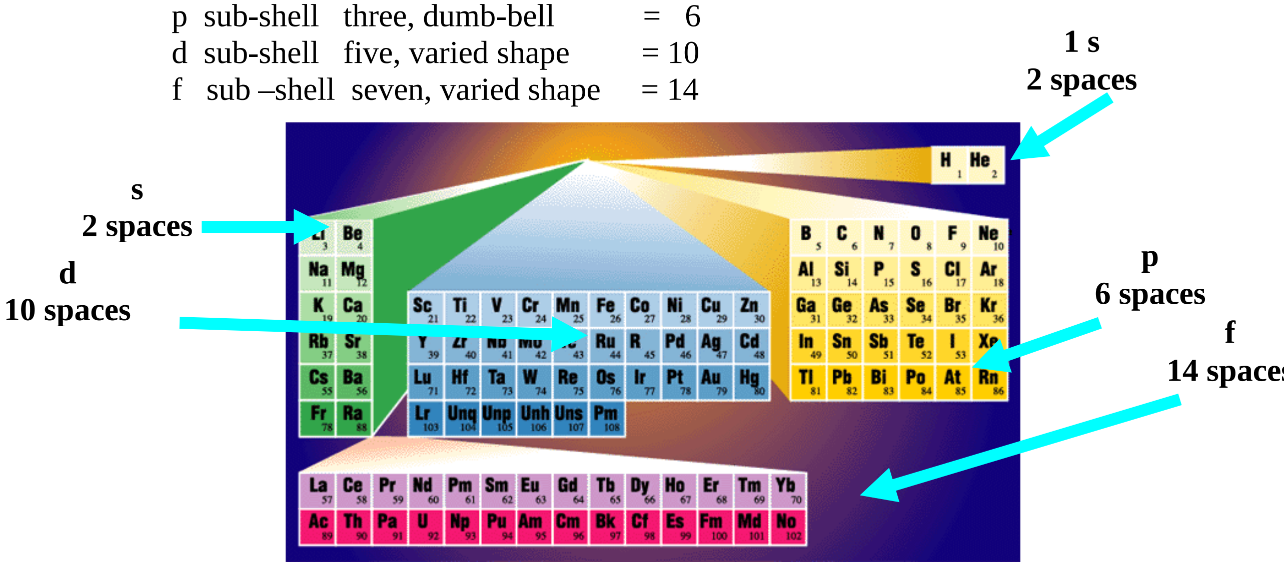
Each orbital gets one electron before accepting a second electron
Orbitals will fill with maximum number of unpaired electrons

For p orbitals

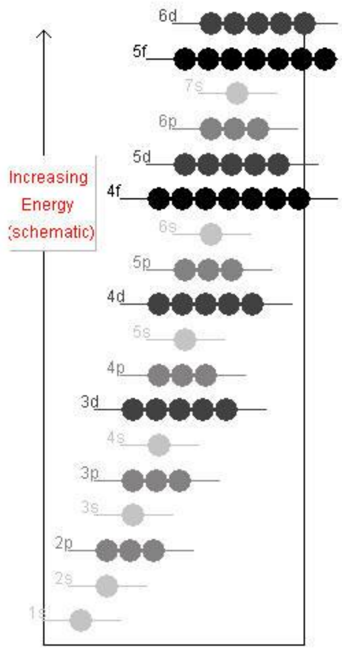
Orbital Occupancy

Since each orbital can have 2 electrons, the maximum occupancy:

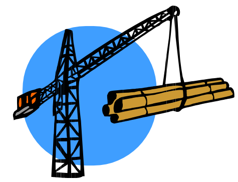
s	sub-shell	one, spherical	= 2
p	sub-shell	three, dumb-bell	= 6
d	sub-shell	five, varied shape	= 10
f	sub –shell	seven, varied shape	= 14

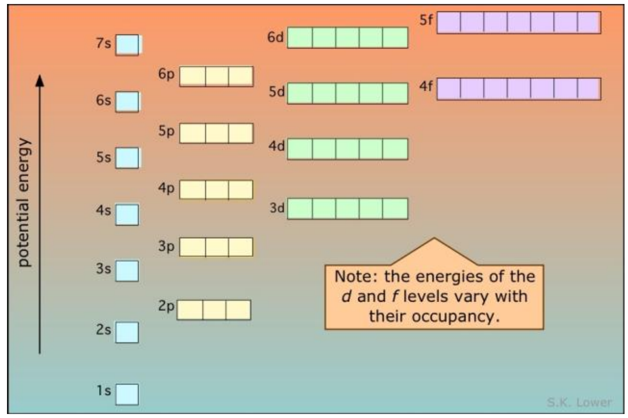


Aufbau Priciple



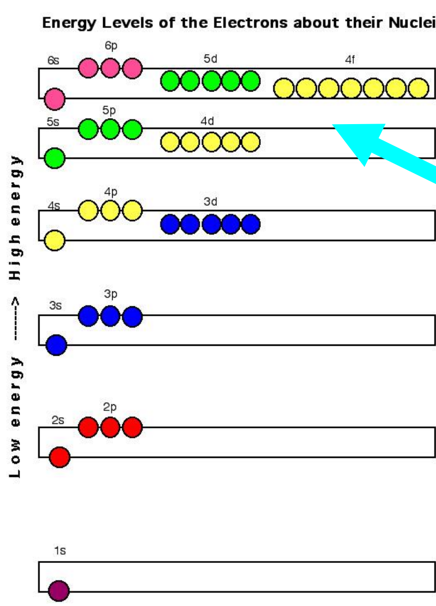
German for "construction" or build-up
Termed coined by Niels Bohr in 1920





Electron Configurations for atoms of Periodic Table are constructed by progressively adding electrons to build the selected atom

Electron Energy Diagram

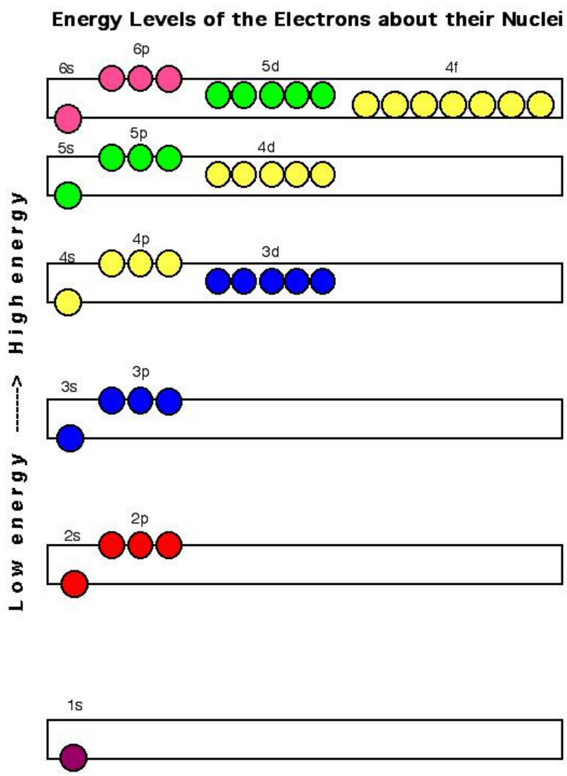


Energies

Large Between n's
Small Between l 's

Small Differences
Allow Multiple Configurations
This Explains
Transition Element
Multiple Oxidation States

Worksheet



Start at lower level

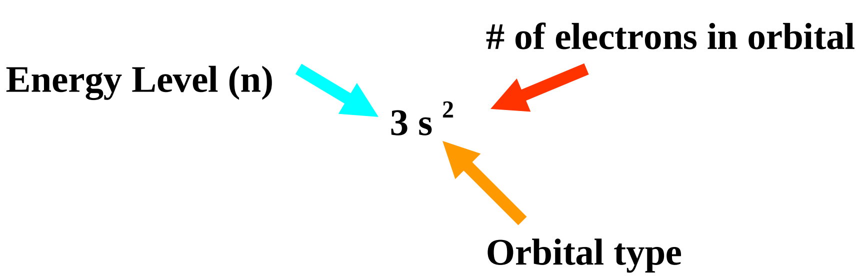
Add electrons
Until correct # reached

2 electrons per orbital

This corresponds to
Periodic Table
Arrangement of Elements

Electron Configuration Nomenclature

Shows sub-shell (orbital) distribution of electrons



Use Periodic Table to list electrons
List electron configuration in order of atomic number
Start with H (Z=1)
Continue adding electrons until desired element is reached

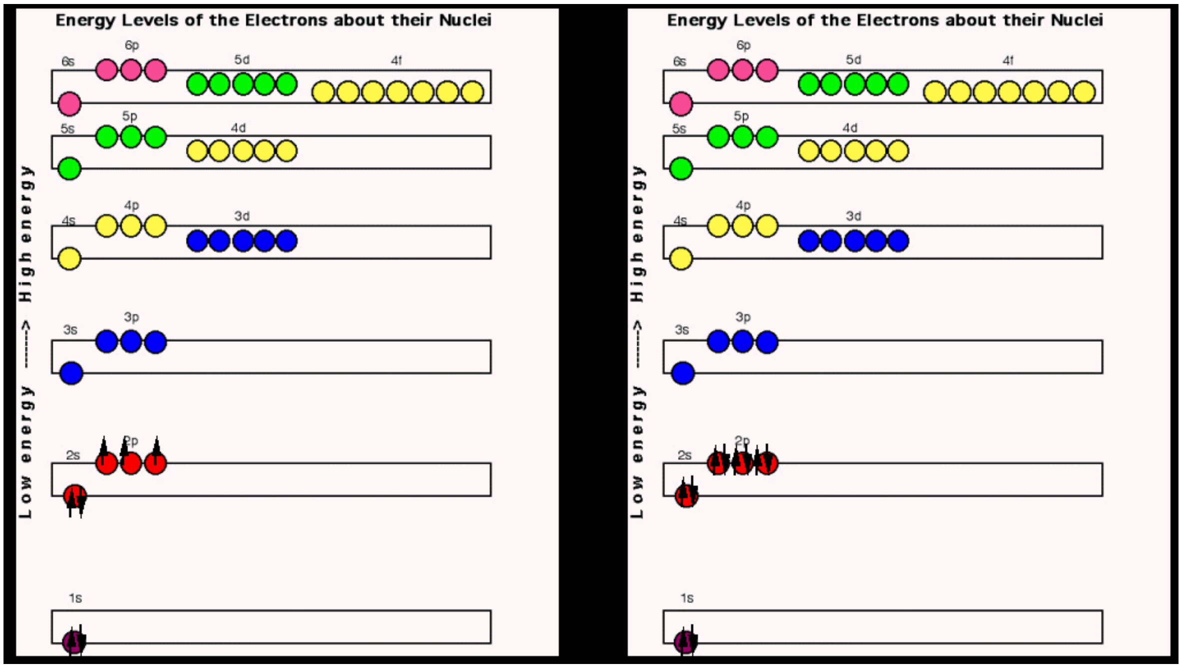
Worksheet - Examples

For Nitrogen (Z= 7)

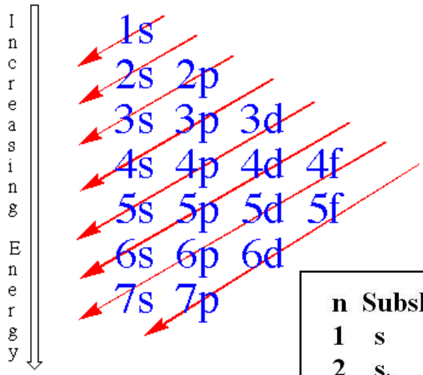
$1s^2\ 2s^2\ 2p^3$

For Neon (Z= 10)

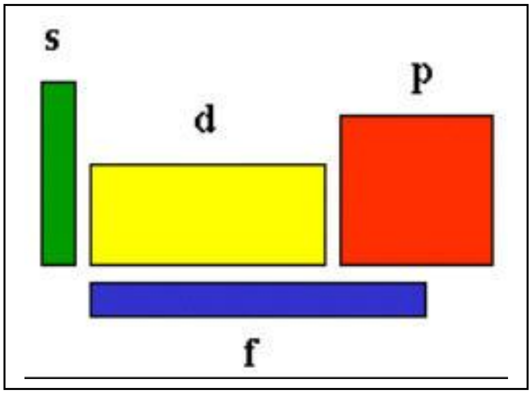
$1s^2\ 2s^2\ 2p^6$

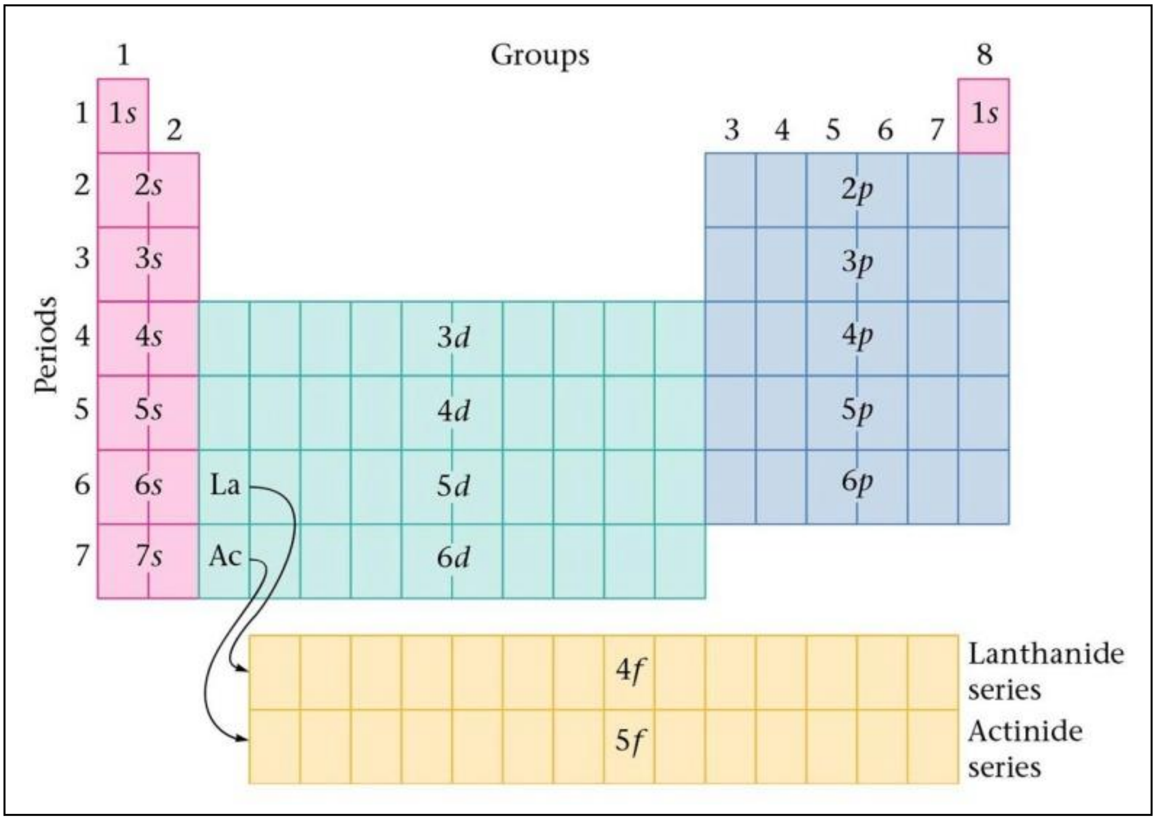


Order of Orbital Filling



n	Subshells (Orbitals)
1	s
2	s, 2p
3	s, 3p
4	s, 3d, 4p
5	s, 4d, 5p
6	s, 4f, 5d, 6p
7	s, 5f, 6d, 7p





Aufbau Principle – Examples

1 H $1s^1$
2 He $1s^2$ = [He]
3 Li [He] $2s^1$
4 Be [He] $2s^2$
5 B [He] $2s^2$ $2p^1$
6 C [He] $2s^2$ $2p^2$
7 N [He] $2s^2$ $2p^3$
8 O [He] $2s^2$ $2p^4$
9 F [He] $2s^2$ $2p^5$
10 Ne [He] $2s^2$ $2p^6$ = [Ne]
11 Na [Ne] $3s^1$
12 Mg [Ne] $3s^2$
13 Al [Ne] $3s^2$ $3p^1$
14 Si [Ne] $3s^2$ $3p^2$
15 P [Ne] $3s^2$ $3p^3$
16 S [Ne] $3s^2$ $3p^4$

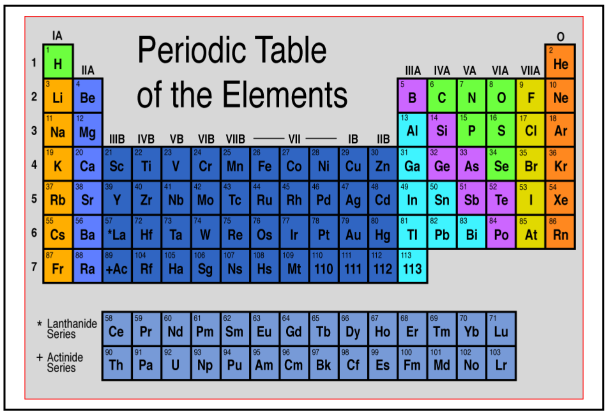
* Exceptions to Aufbau

20 Ca [Ar] $4s^2$
21 Sc [Ar] $4s^2$ $3d^1$
22 Ti [Ar] $4s^2$ $3d^2$
23 V [Ar] $4s^2$ $3d^3$
24 Cr [Ar] $4s^1$ $3d^5$*
25 Mn [Ar] $4s^2$ $3d^5$
26 Fe [Ar] $4s^2$ $3d^6$
27 Co [Ar] $4s^2$ $3d^7$
28 Ni [Ar] $4s^2$ $3d^8$
29 Cu [Ar] $4s^1$ $3d^{10}$*
30 Zn [Ar] $4s^2$ $3d^{10}$
31 Ga [Ar] $4s^2$ $3d^{10}$ $4p^1$
32 Ge [Ar] $4s^2$ $3d^{10}$ $4p^2$
33 As [Ar] $4s^2$ $3d^{10}$ $4p^3$
34 Se [Ar] $4s^2$ $3d^{10}$ $4p^4$
35 Br [Ar] $4s^2$ $3d^{10}$ $4p^5$
36 Kr [Ar] $4s^2$ $3d^{10}$ $4p^6$

Periodic Table – Summary of Families

Periodicity (Columns) a Function of Similar Outer Shell

Group 1A (1): alkali metals
Group 2A (2): alkaline earth metals
Group 7A (17): halogens
Group 8A (18): noble (inert) gases
Representative (1-2;13-18): The A Groups (the Edges)
Transition Metals (3-12): The B Groups (the Center)
Metalloids: "Staircase" B,Si, Ge, As, Sb, Te, Po



Lanthanides = upper, of lower rows
Actinides = lower, of lower row

Predicted Chemical Properties
Elements in the same column are similar
Elements in different columns are different

Valence electrons

Highest energy level (Outer-most shell)
Representative elements involve s or p orbitals
Maximum number for s + p orbitals = eight (the "octet")
Periodic Table columns (Families) = same # valence electrons
Valence electrons determine chemical properties

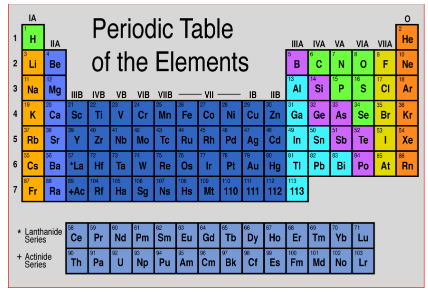
Family	**Outer Shell**
Group1A	**ns^1**
Group 2A	**ns^2**
Group 3A	**ns^2np^1**
Group 4A	**ns^2np^2**
Group 5A	**ns^2np^3**
Group 6A	**ns^2np^4**
Group 7A	**ns^2np^5**
Group 8A	**ns^2np^6**

Isoelectronic Atoms

Monatomic Ions With Noble Gas Electron Configurations
Isoelectronic = identical electron configuration
Atoms form ions to obtain a noble gas electron configuration

Na $1s^2 2s^2 2p^6 3s^1$
Na^+ $1s^2 2s^2 2p^6$
Ne $1s^2 2s^2 2p^6$ > Isoelectronic

O $1s^2 2s^2 2p^4$
O^{2-} $1s^2 2s^2 2p^6$
Ne $1s^2 2s^2 2p^6$ > Isoelectronic
Atoms gain or lose electrons
To acquire a noble configuration



Any Atom pair with the same electronic configuration is isoelectronic

Ne, F^-, O^{2-} are isoelectronic
Ar, Cl^-, S^{2-} are isoelectronic

Mg^{2+} , Na^+ , Ne are isoelectronic
Ca^{2+} , K^+ , Ar are isoelectronic

Assignment

Start Taking Unit 10 Practice Test
The Practice Quiz is very similar to the Unit Exam
Success on Unit exam is directly related to practice exam experience