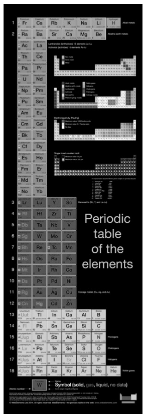
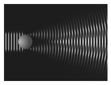
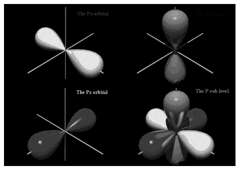
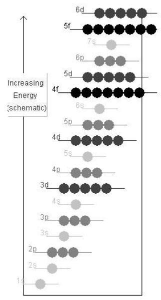
Atomic Theory









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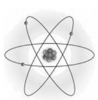
Atomic Theory

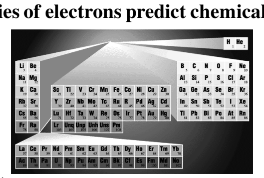


At the particulate (atomic) level:

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



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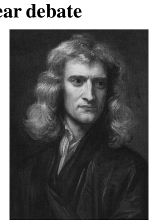
Modern Atomic Theory

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 **Isaac Newton**

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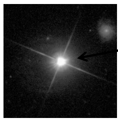
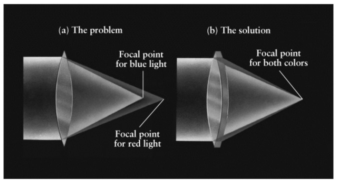
Problem: Need Method to Remove Color Blurring



Should be single point



Need to understand light
To improve lens design

Particles vs waves:
Different math

Modern lenses have 5 or more optical elements

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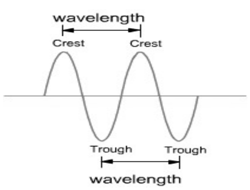
Particles vs. Waves

Particles = like tiny BB's

Wave = repeating oscillation

Wavelength (λ) = distance between adjacent identical points
Frequency (ν) = # 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"

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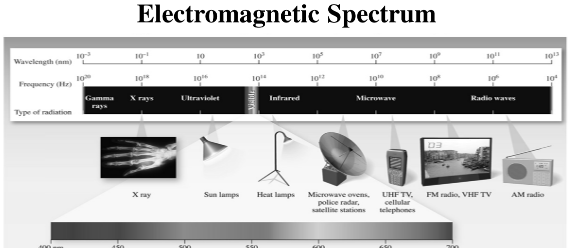
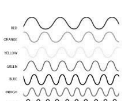
Electromagnetic Spectrum



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**



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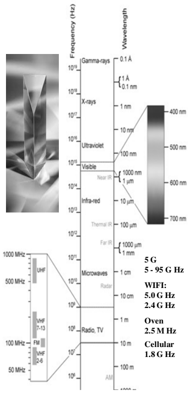
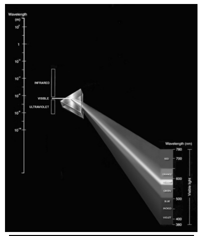
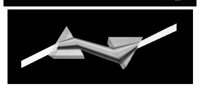


Visible Light

Only a small portion
Of
Electro-magnetic spectrum





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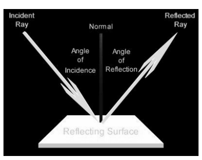
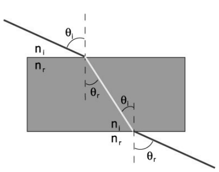
Properties of Light



Reflection

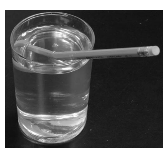
Mirrors



Refraction

Bending

Lenses



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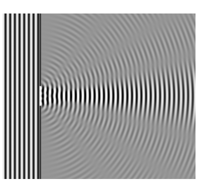
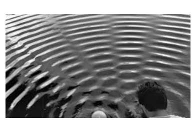
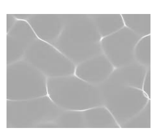
Properties of Light

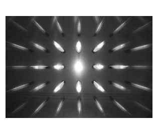


Interference

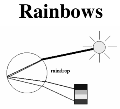


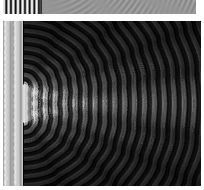
Amplification
Cancellation





Diffraction
Prisms
Rainbows





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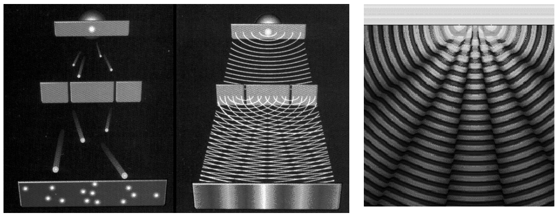
Properties of Light

Two-Slit Experiment
Attempt to Measure Alters Results



2 Slits Emphasize Interference (wave phenomena)
Try to measure at slits: get no interference, just particle pattern

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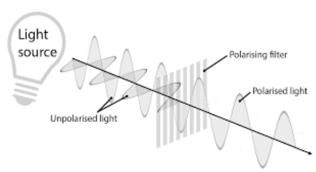
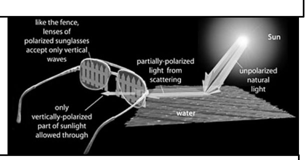
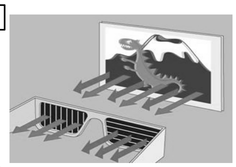
Properties of Light

Polarization



Glare Filters
3-D Visualizations
Strain Visualizations





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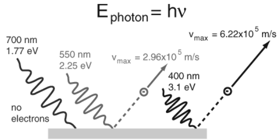
Properties of Light

Photoelectric Effect – light creates current (electrons) flow

$E_{photon} = h\nu$

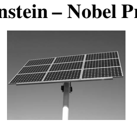


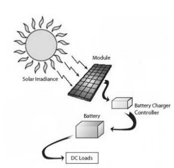
Photoelectric effect

Not all colors (energies)
Create photoelectric effect

Only Possible by
Energy transfer of particles

Einstein – Nobel Prize





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Properties of Light

Summary

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

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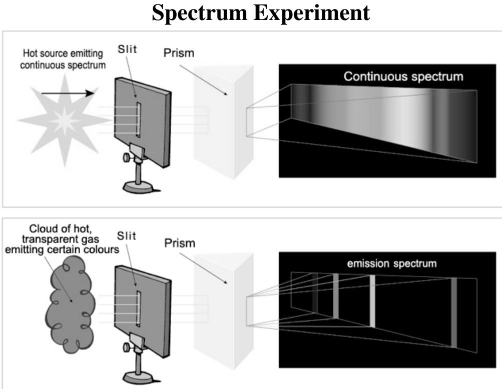
Spectrum Experiment



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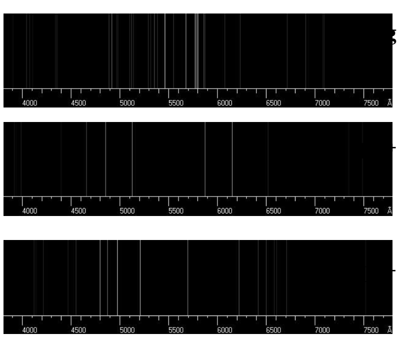
Emission Spectra: Measure of electron energy



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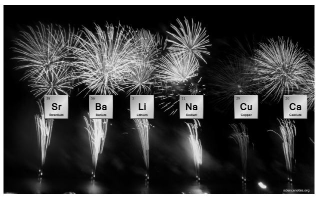
Emission Spectra

Determines Observed Colors

Of Lights & Flames

Na Vapor

Hg Vapor



Pyrotechnics

Aurora's

Red: Oxygen
Blue Green Purple: Nitrogen

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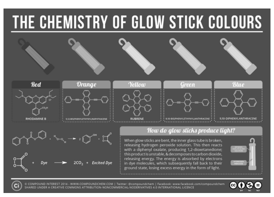
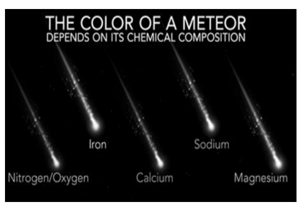
Emission Spectra

Determines Observed Colors Of lights & flames





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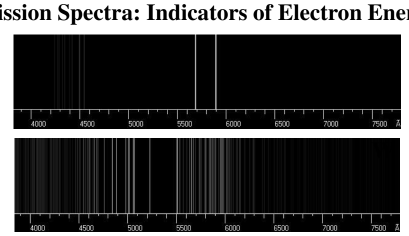
Emission Spectra: Indicators of Electron Energy



Emission spectra – Discrete energy lines
Define electron energies
Different electron energies
Define chemical properties
Define Periodic Table Arrangement

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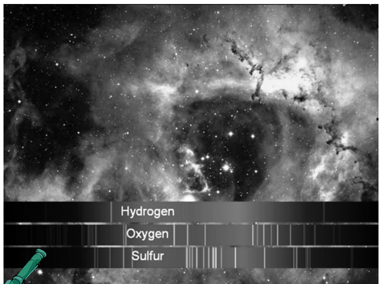
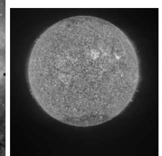
Emission Spectra: Astronomical Tool for Discovery





Presence of Hydrogen and Oxygen Exciting

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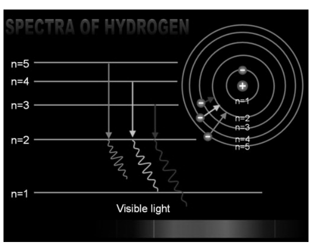
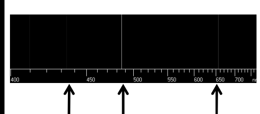
Electron States





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

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

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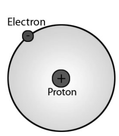
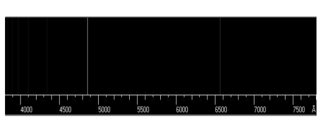
Bohr Model of the Hydrogen Atom

Treated electron as a particle
Energies of electrons are quantized (discrete steps)
Electrons 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



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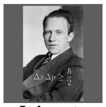
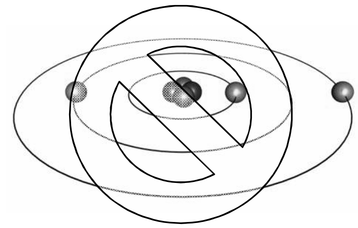


Heisenberg Uncertainty Principle

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)

At the atomic level,



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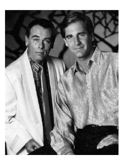
Modern Atomic Theory (Quantum Mechanics)

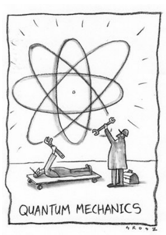
Wave-Particle Duality

Explaining light and sub-atomic particles requires duality

Quantum Mechanics
Discrete, non-continuous values of energy

Energy "Leaps" from one level to another





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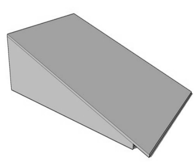
Quantum Means "In Discrete Steps"



Quantized Process **Continuous Process**

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Quantum Mechanics

Schrödinger (1925) Wave Equation

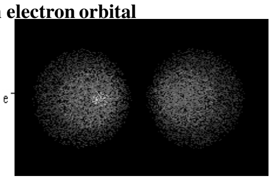
H Ψ = E Ψ

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

Ψ^2 gives probability of finding an electron in space
So, Ψ^2 plot defines an electron orbital

Selected Ψ function (p orbital)

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



Each electron: separate equation

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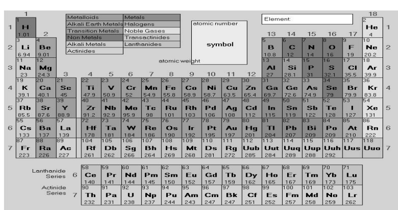
Quantum Mechanics

Schrödinger Wave Equation Solution
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



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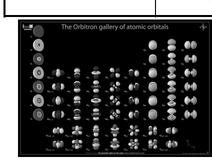
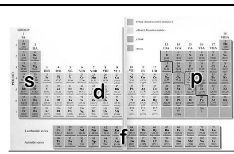
Quantum Numbers

Name	Symbol	Meaning
Principle	n	Shell
Azimuthal	ℓ	Orbital Type
Magnetic	m_ℓ	Orbital Orientation
Spin	m_s	Spin





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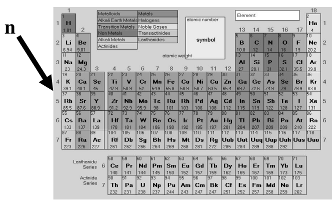
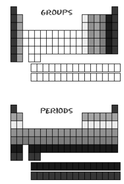
Principle Quantum Number (n)

Value of n = 1, 2, 3, …, ∞

Represents average energy of electron orbital
Increasing n ➔ increasing energy
Increasing n ➔ increasing distance from the nucleus
Corresponds to the n value (row) on the periodic table
Corresponds to number of sub-orbitals available
Maximum number of electrons per n = $2n^2$





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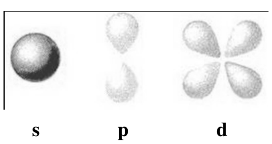
Azimuthal Quantum Number (ℓ)

Value of $0 \le \ell \le n-1$

Represents Sub-Orbital Type
$\ell = 0$ ➔ s orbital (spherical) "sharp"
$\ell = 1$ ➔ p orbital (dumb-bell) "principal"
$\ell = 2$ ➔ d orbital (varied shape) "diffuse"
$\ell = 3$ ➔ f orbital (varied shape) "fundamental"



Electron Shell (n)	Subshells Available	Orbitals Available ($2\ell + 1$)
1	s	1
2	s	1
	p	3
3	s	1
	p	3
	d	5
4	s	1
	p	3
	d	5
	f	7

Max # electrons per $\ell = 4\ell + 2$

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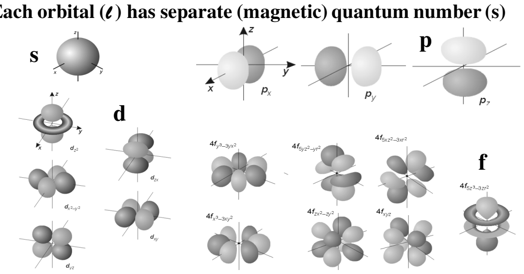
Magnetic Quantum Number (m_ℓ)

Value of $-\ell \le m_l \le \ell$

Represents spatial orientation (with respect to external field)
Corresponds to probability of finding electron
Each orbital (ℓ) has separate (magnetic) quantum number (s)



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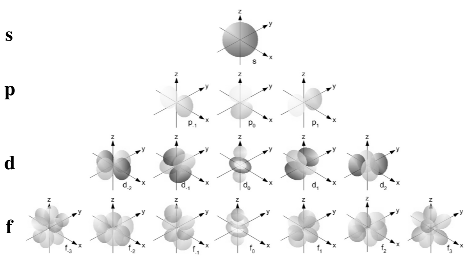
Planets Travel in Orbits
Electrons Occupy Orbitals



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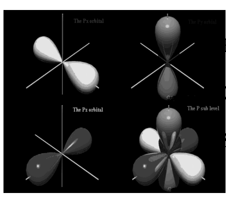
Pauli Exclusion Principle

Based on observation of spectral lines (energy)
Maximum 2 electrons per orbital
No two electrons have same set of quantum numbers



Each p orbital can have max 2 electrons

Composite (each shell, n) has

3 orbitals x $\frac{\text{2 electrons}}{\text{orbital}}$ = 6 electrons

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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

Based on observations of spectral energy
Each orbital gets one electron before accepting a second
Orbitals will fill with maximum number of unpaired electrons

For P Orbitals

↑ ↑ ↑

Never

↑↑ ↑ _ ↑↓ ↑ _

Like people on a bus:
No one wants
to sit next to another

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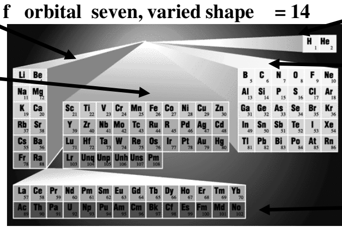
Orbital Occupancy

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

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



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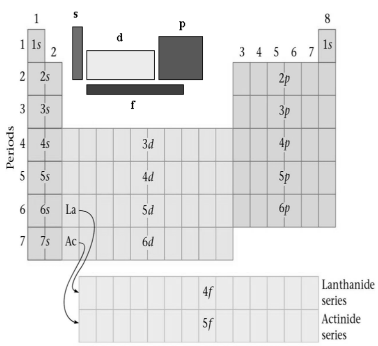
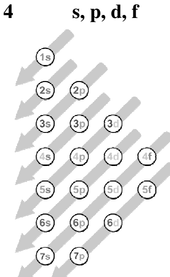
Orbital Filling



Period	Orbitals
1	s
2	s, p
3	s, p, d
4	s, p, d, f



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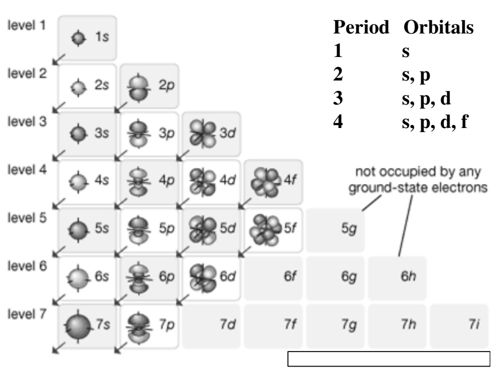
Available Orbitals



Period	Orbitals
1	s
2	s, p
3	s, p, d
4	s, p, d, f

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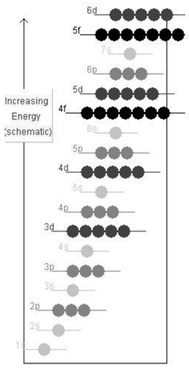
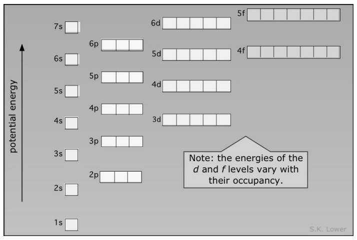


Aufbau Principle

German for "construction" or build-up
Termed coined by Niels Bohr in 1920
Electron Configurations constructed by progressively adding electrons



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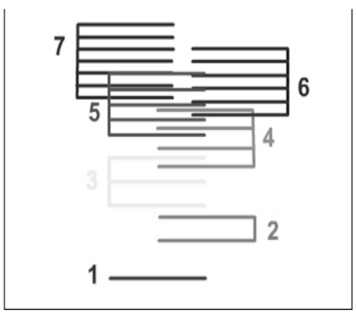
The Orbital Energies Overlap Explains Transition Metal Valence Variability



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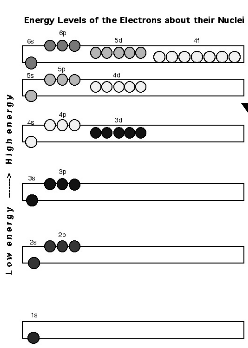
Electron Energy Diagram



Energies

Large Between n's
Small Between ℓ's

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

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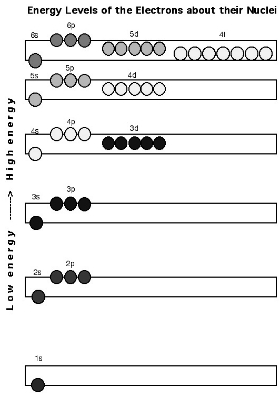

Worksheet

Start at lower level

Add electrons
Until correct # reached

2 electrons per orbital

This corresponds to Periodic Table Arrangement of Elements

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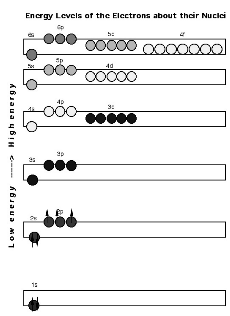
Worksheet - Examples

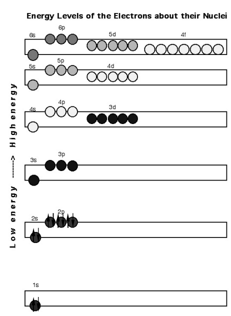
For Nitrogen (Z= 7)

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



For Neon (Z= 10)

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



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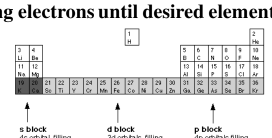
Electron Configuration Nomenclature

Shows sub-shell (orbital) distribution of electrons

# of electrons in orbital

Energy Level (n) → $3s^2$ ← **Orbital type**

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



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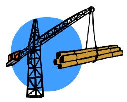
Aufbau Principle - Examples



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] $3s^2\ 3p^4$
17 Cl [Ne] $3s^2\ 3p^5$
18 Ar [Ne] $3s^2\ 3p^6$ = [Ar]
19 K [Ar] $4s^1$

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] $4s^2\ 3d^{10}\ 4p^6$

* Exceptions to Aufbau

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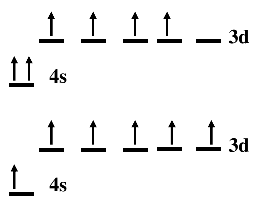
Aufbau Exceptions

Full or exactly half-filled sub-orbitals energetically favorable
Creates 3d-4s exceptions to Aufbau

Cr (Z=24) should have [Ar]$4s^2 3d^4$

But, half-filled stability over-rides:
[Ar]$4s^1 3d^5$



Cu (Z = 29) also promotes a 4s electron to completely fill the 3d

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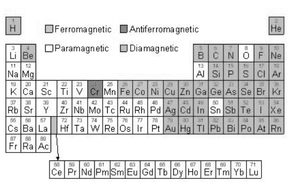
Electron Pairing Affects Magnetic Properties

Paramagnetic elements
Unpaired electrons attracted to magnetic fields
Diamagnetic elements
Paired electrons slightly repelled by magnetic fields
Ferromagnetic
Elements having very high magnetic properties



Magnitude affected by:
Magnetic field strength
Temperature

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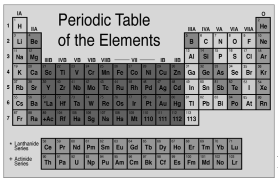
Periodic Table – Summary of Families

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

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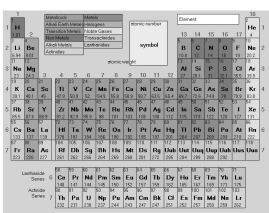
Valence electrons

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

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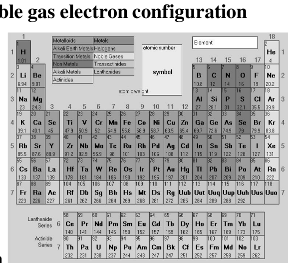
Isoelectronic Atoms

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

Na	$1s^22s^22p^63s^1$
Na^+	$1s^22s^22p^6$]
Ne	$1s^22s^22p^6$]
O	$1s^22s^22p^4$
O^{2-}	$1s^22s^22p^6$]
Ne	$1s^22s^22p^6$]

Isoelectronic



Atoms gain or lose electrons
To acquire a noble configuration

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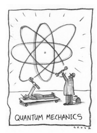
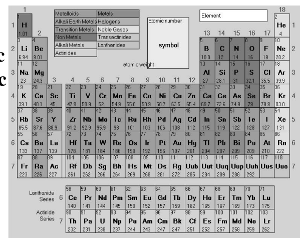
Isoelectronic Atoms

Any pair of atoms 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





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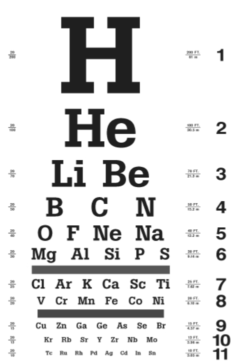
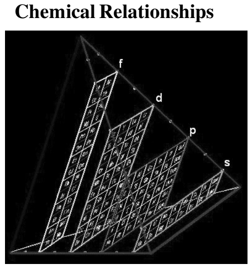


Bottom Line:
Knowledge of the Periodic Table Allows You To See All Sorts of Chemical Relationships



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