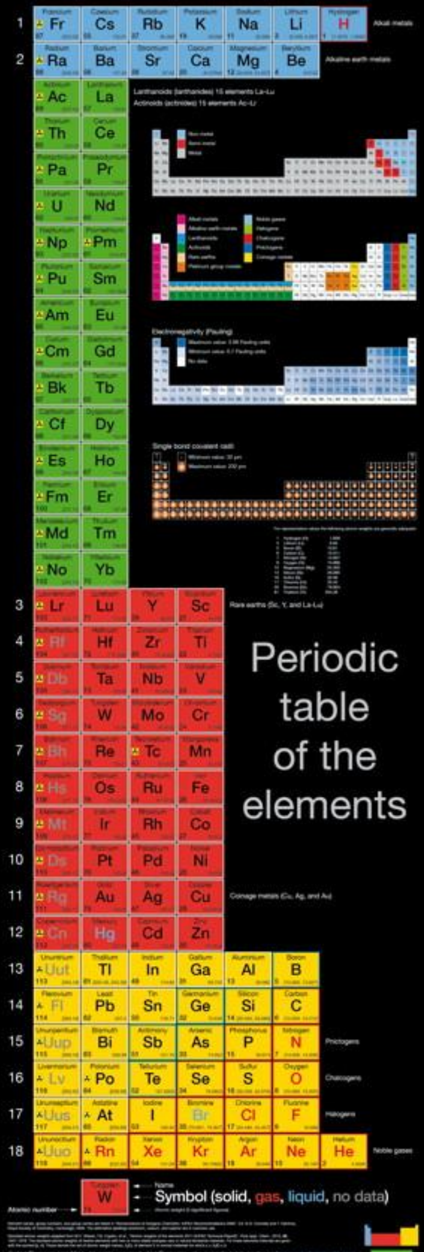
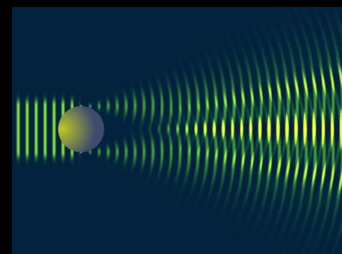
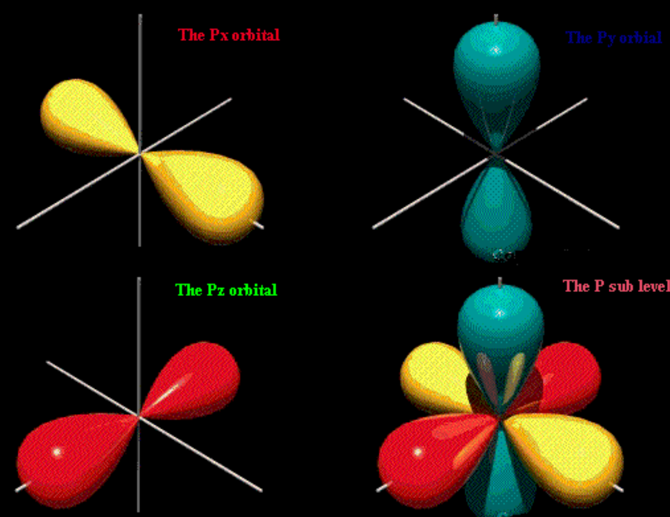
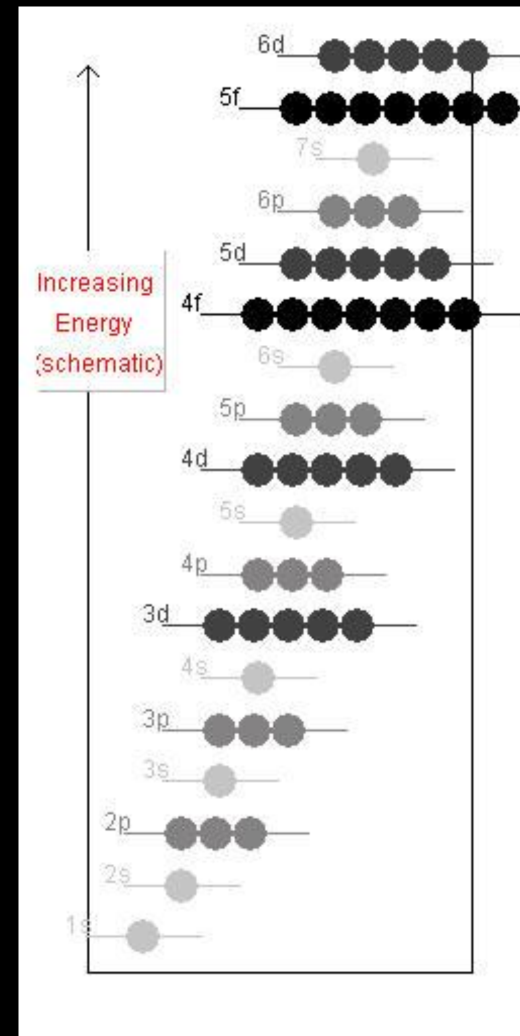
Atomic Theory









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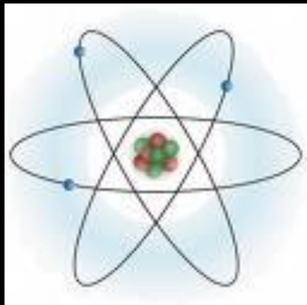


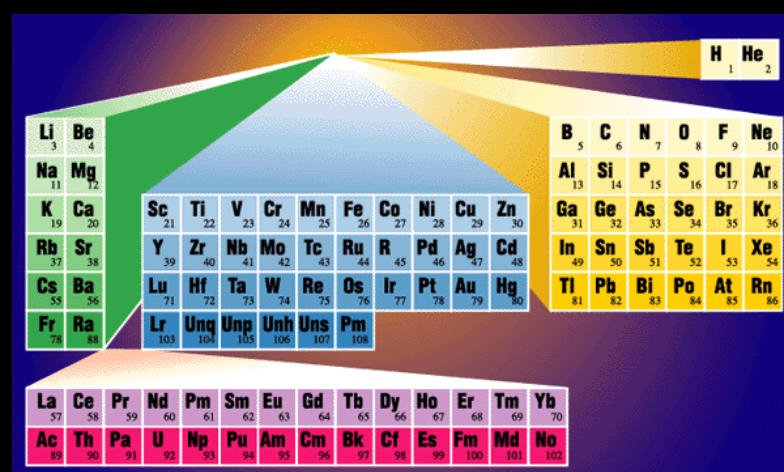
Atomic Theory

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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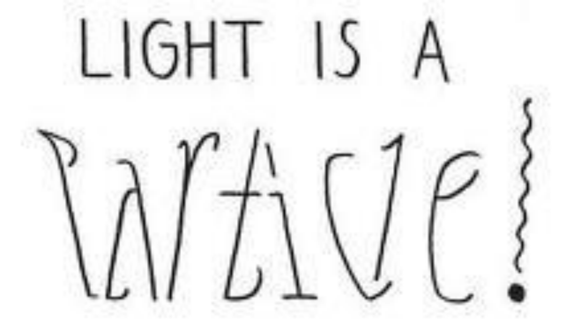
Modern Atomic Theory

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

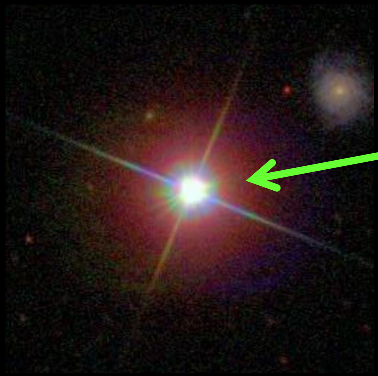
Quantum Theory emerged after 300 year debate

Light
Wave or Particle?

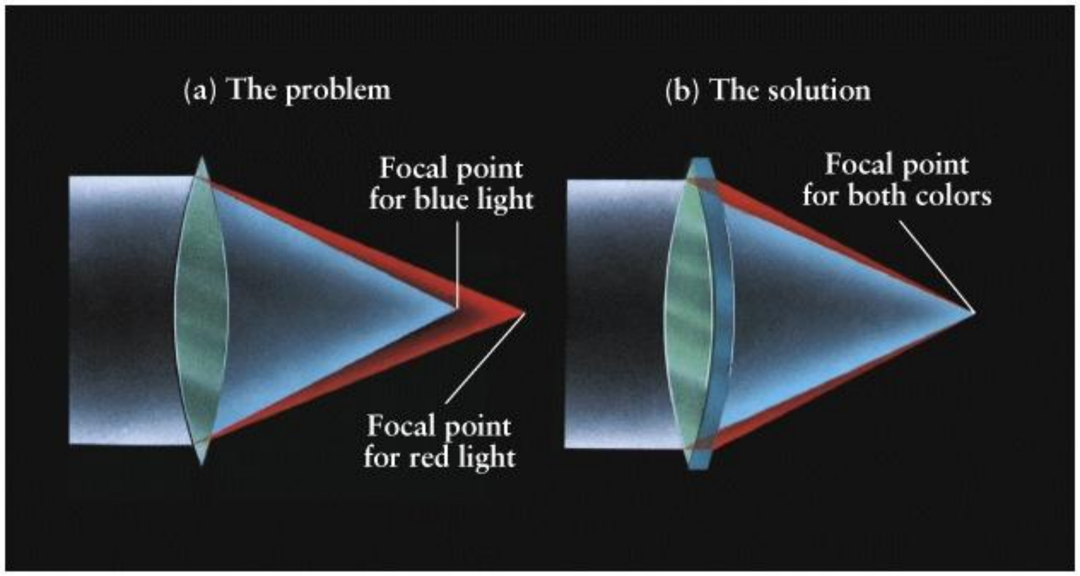


Christian Huygens **Isaac Newton**

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

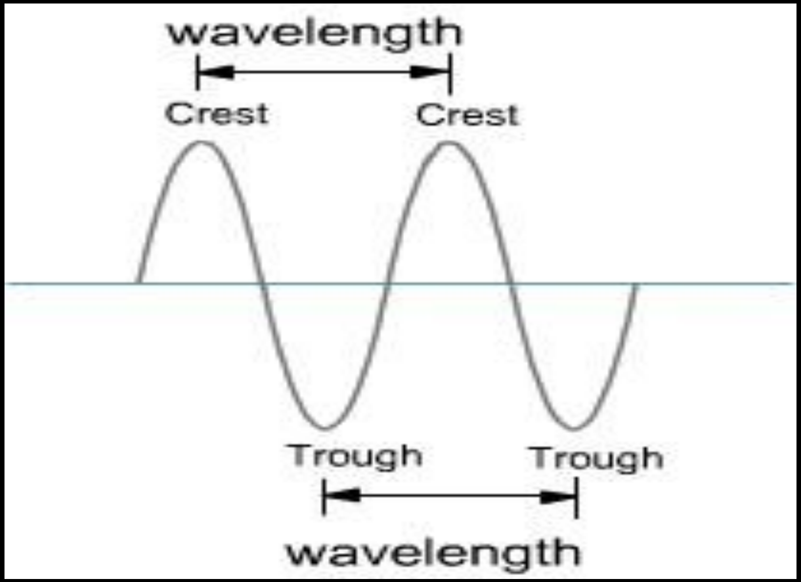
Wavelength (λ) = distance between adjacent identical points

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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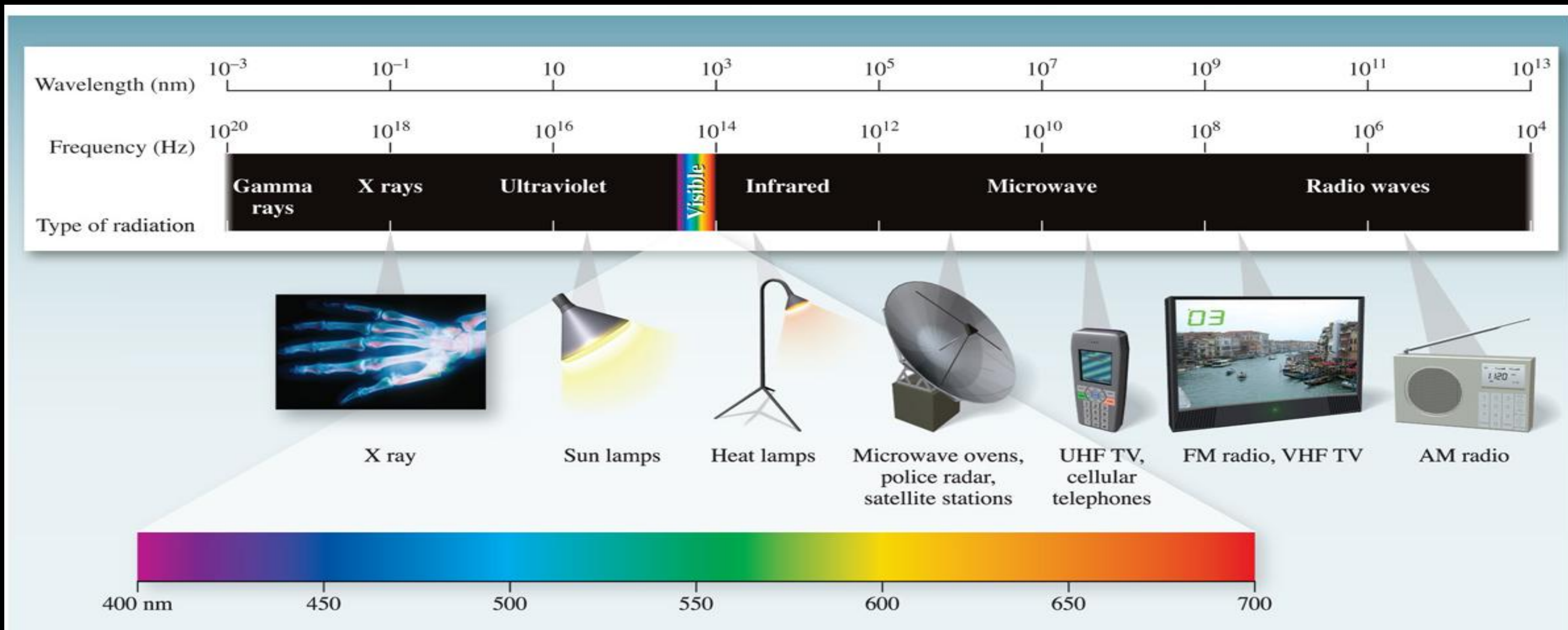
Electromagnetic Spectrum



Wave energy & frequency are directly related.

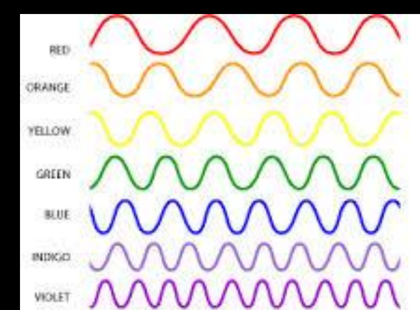
frequency increases, energy increases

energy decreases, frequency decreases

Wave energy & wavelength are inversely related

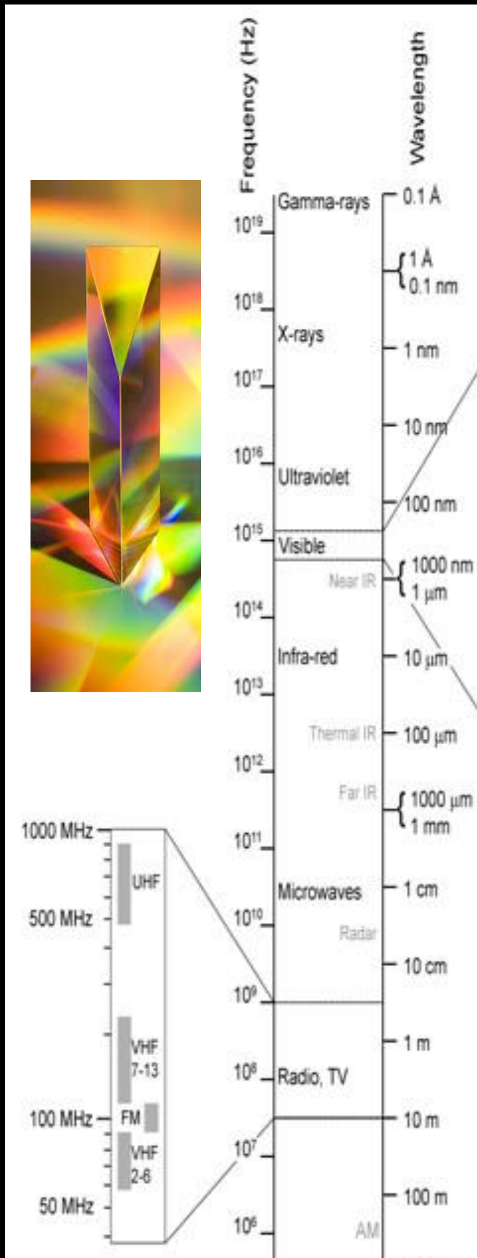
wavelength increases, energy decreases

wavelength decreases, energy increases



Visible Light

Only a small portion
Of
Electro-magnetic spectrum

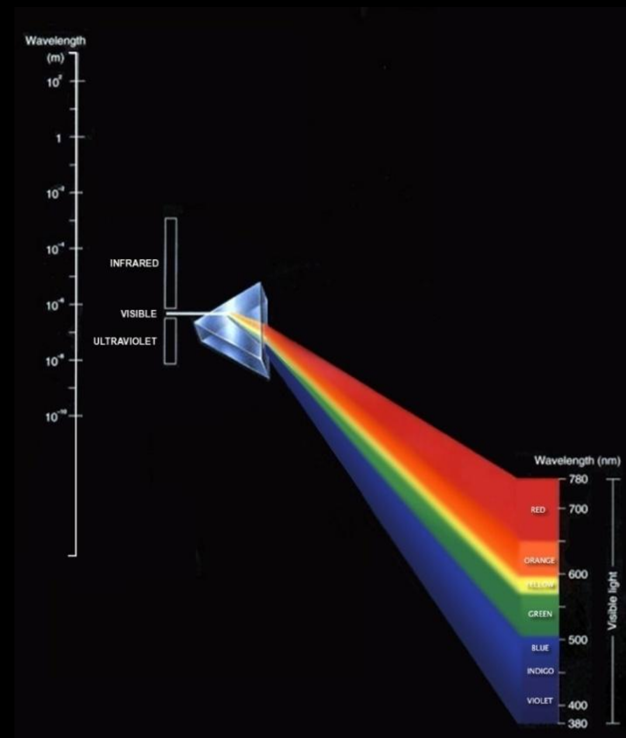


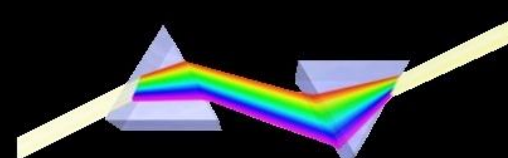
5 G
5 - 95 G Hz

WIFI:
5.0 G Hz
2.4 G Hz

Oven
2.5 M Hz

Cellular
1.8 G Hz





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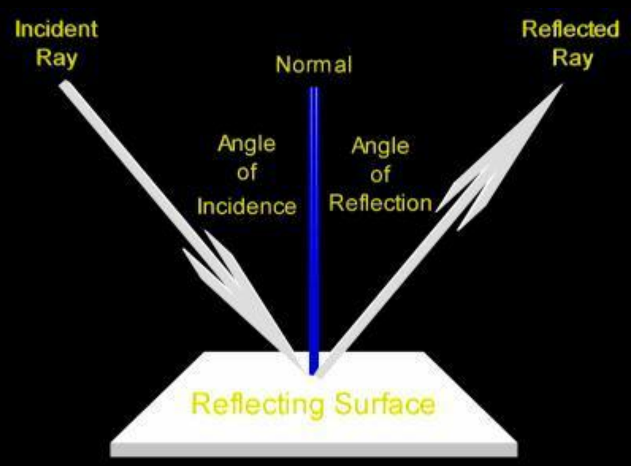
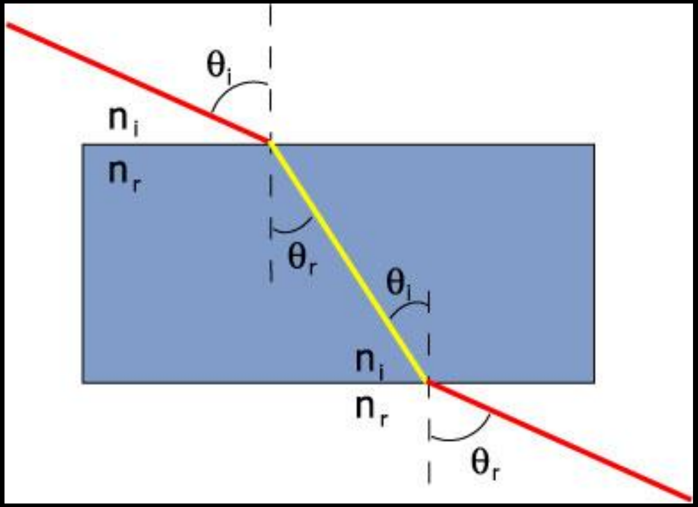
Properties of Light



Reflection

Mirrors

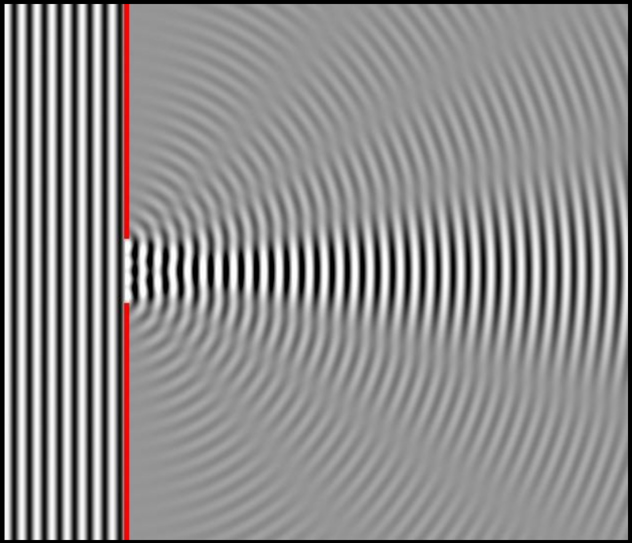


Refraction

Bending

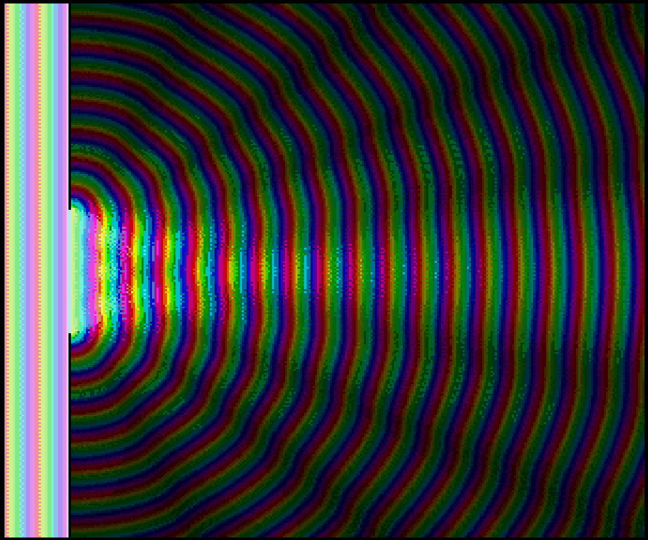
Lenses

Properties of Light



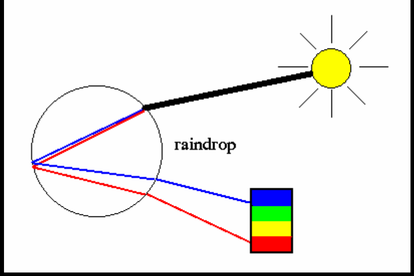
Interference

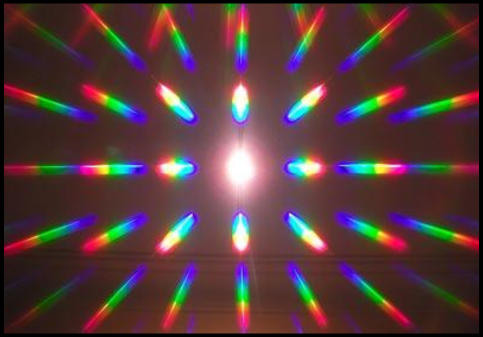
Amplification
Cancellation



Diffraction

Prisms
Rainbows





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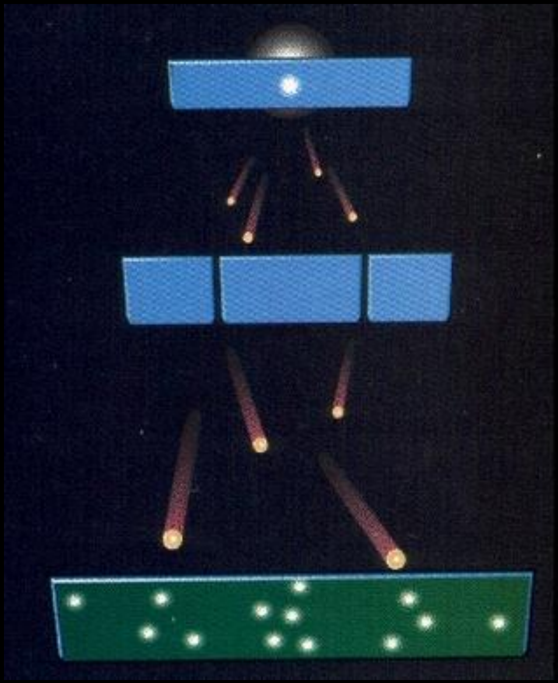
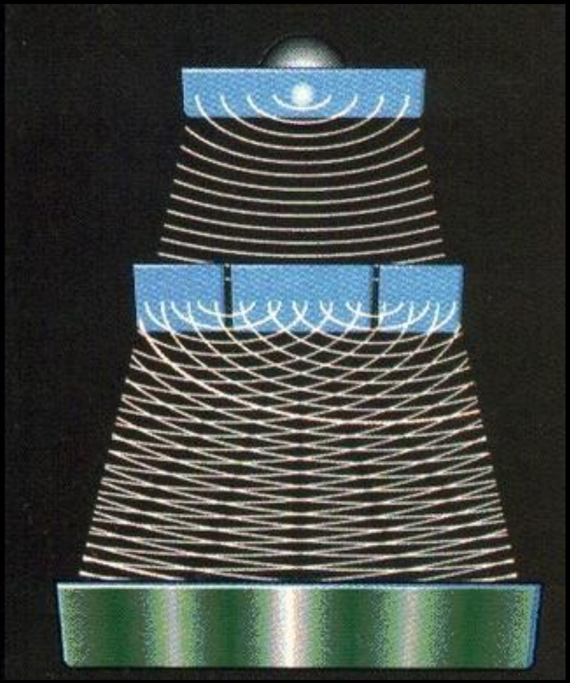
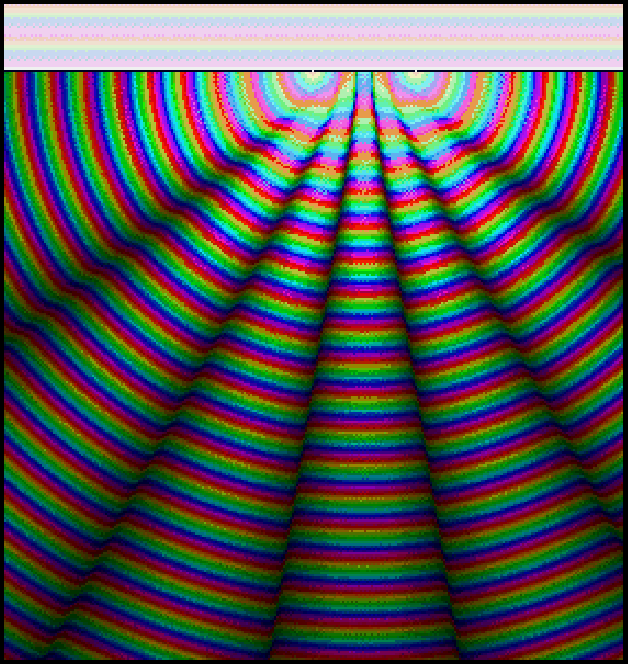
Properties of Light

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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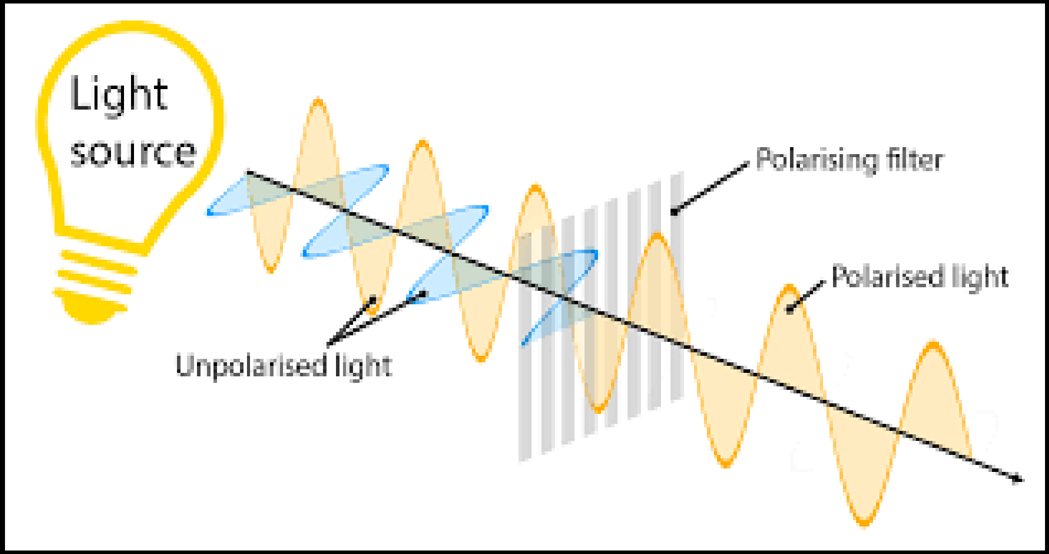
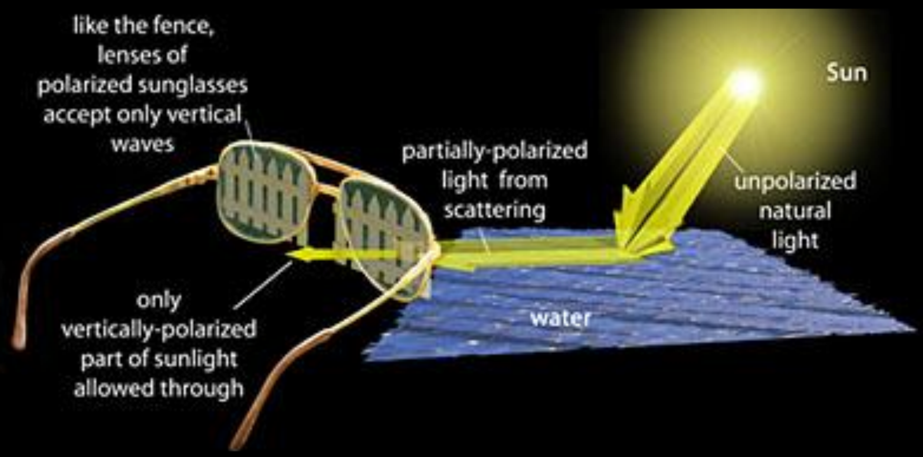
Properties of Light

Polarization



Glare Filters
3-D Visualizations
Strain Visualizations



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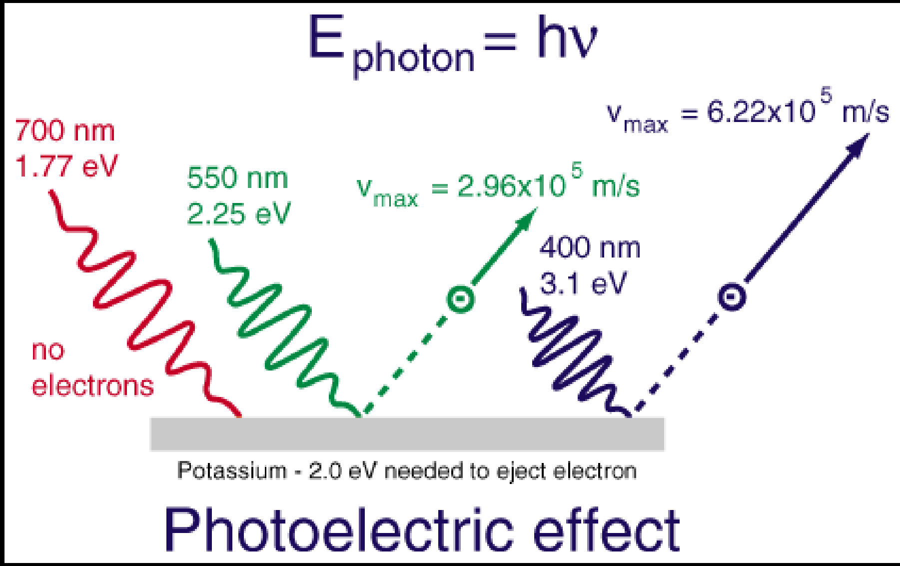
Properties of Light

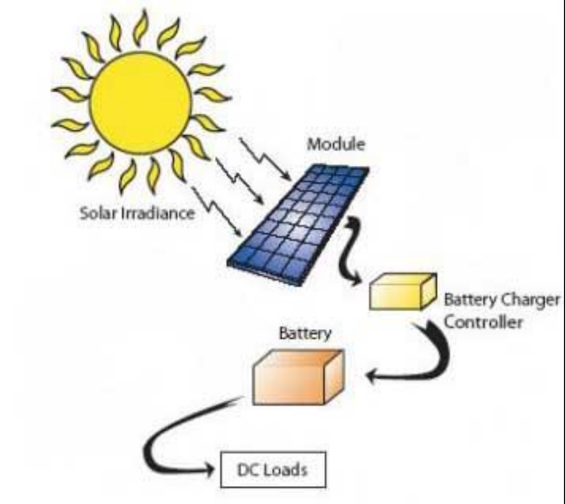
Photoelectric Effect – light creates current (electrons) flow



Not all colors (energies) Create photoelectric effect

Only Possible by Energy transfer of particles

Einstein – Nobel Prize



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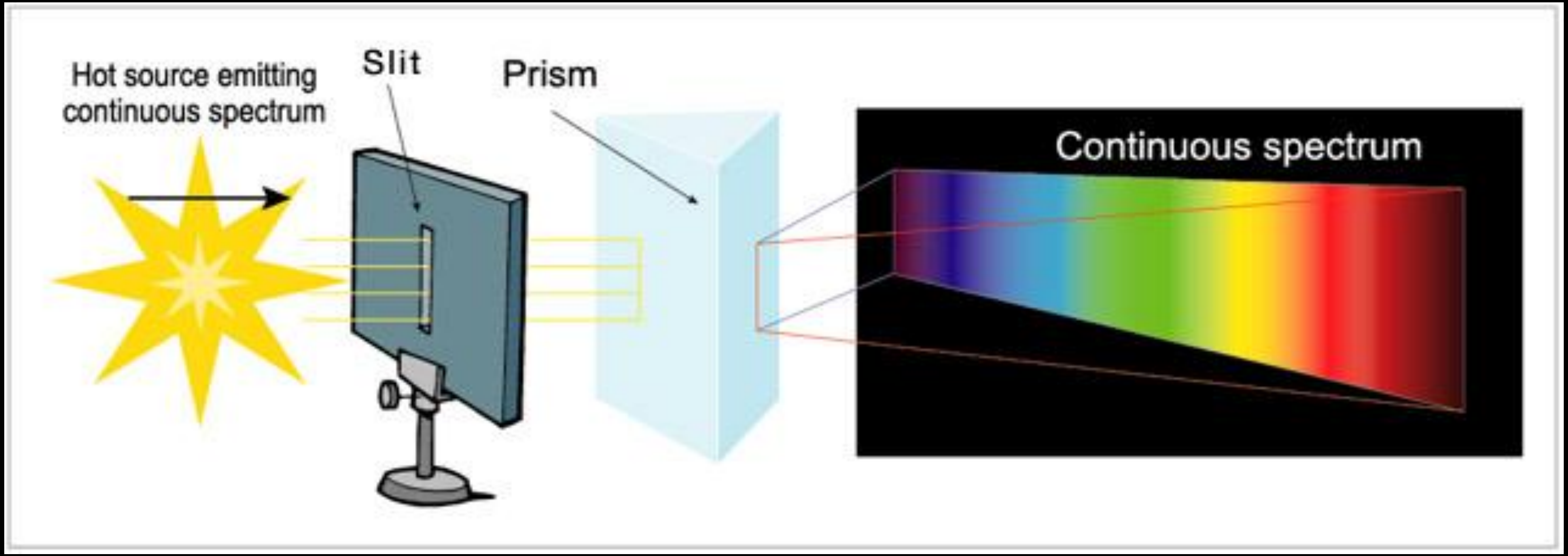
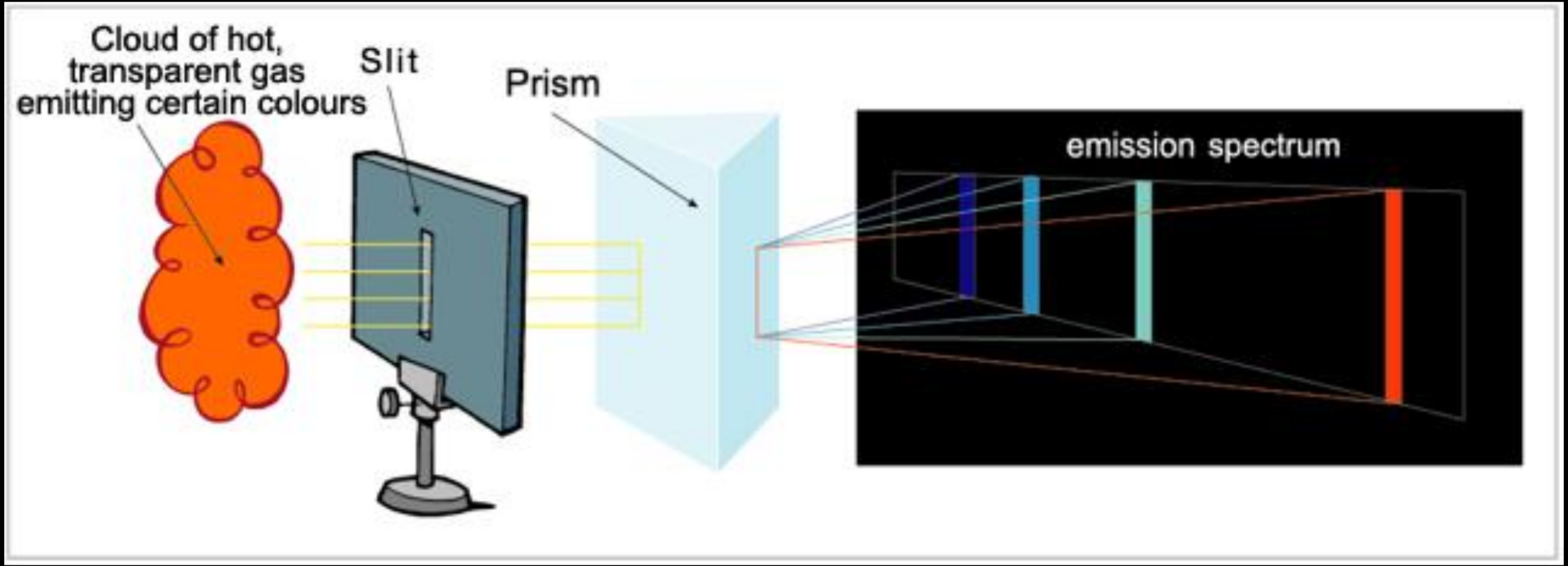
Properties of Light

Summary

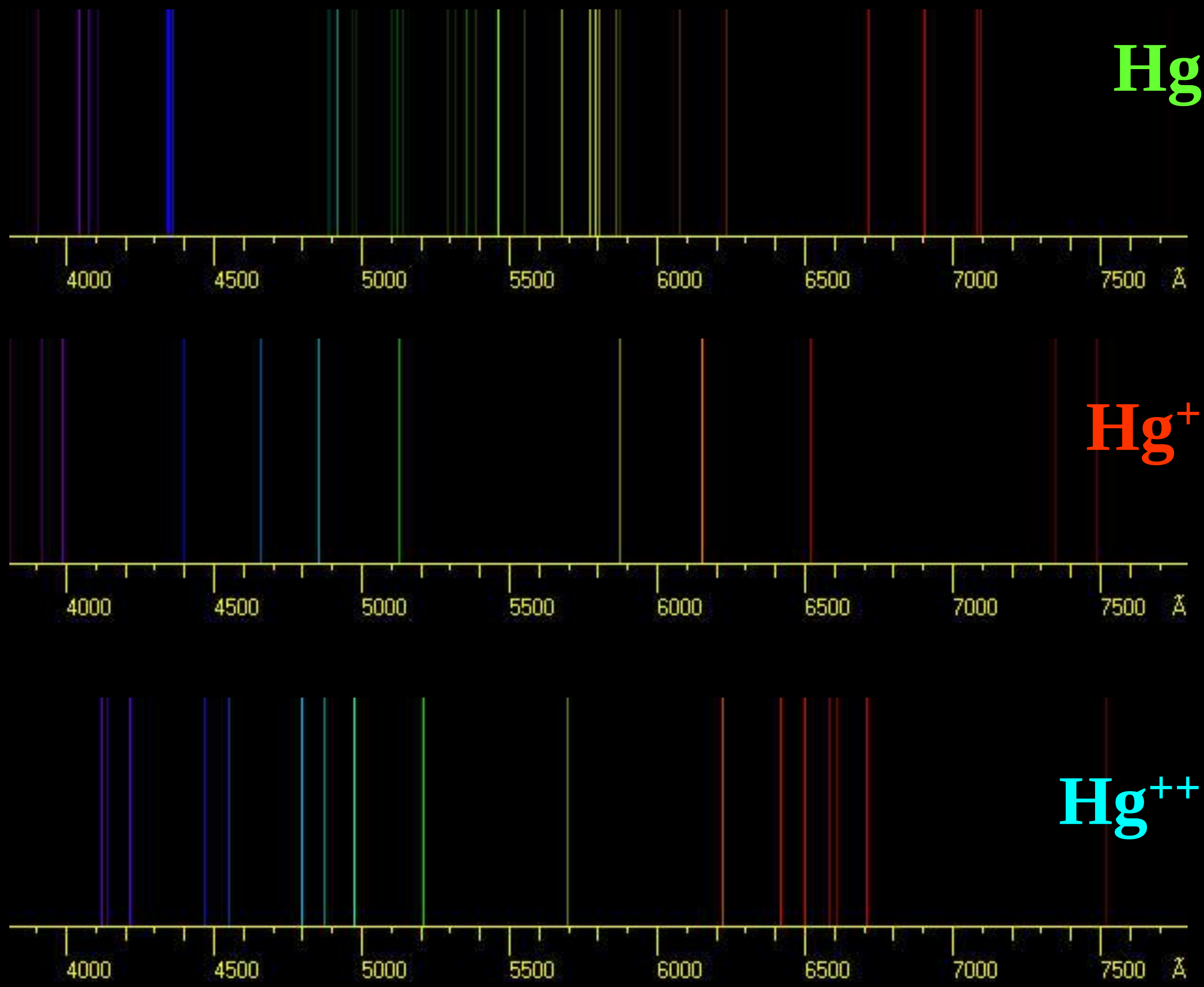
Phenomenon	Can be explained in terms of waves.	Can be explained in terms of particles.
Reflection	✓	✓
Refraction	✓	✓
Interference	✓	⊗
Diffraction	✓	⊗
Polarization	✓	⊗
Photoelectric effect	⊗	✓

Spectrum Experiment





Emission Spectra: Measure of electron energy



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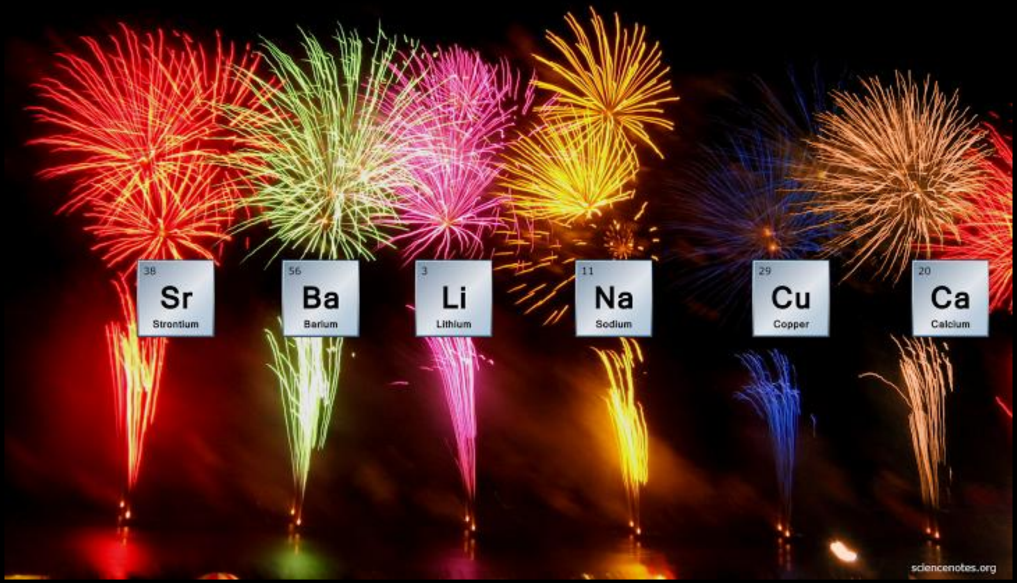
Emission Spectra

Determines Observed Colors

Of Lights & Flames

Na Vapor

Hg Vapor



Pyrotechnics

Aurora's

Red: Oxygen

Blue Green Purple: Nitrogen

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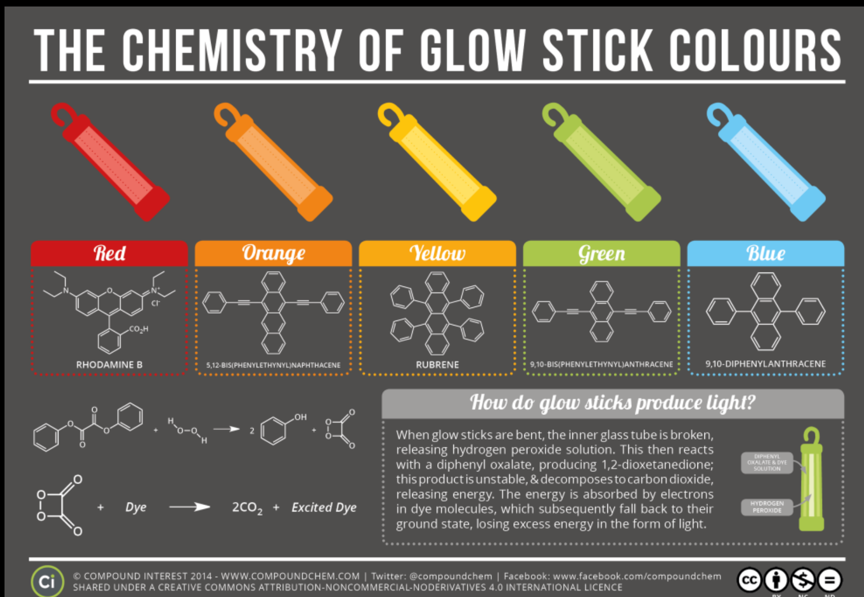
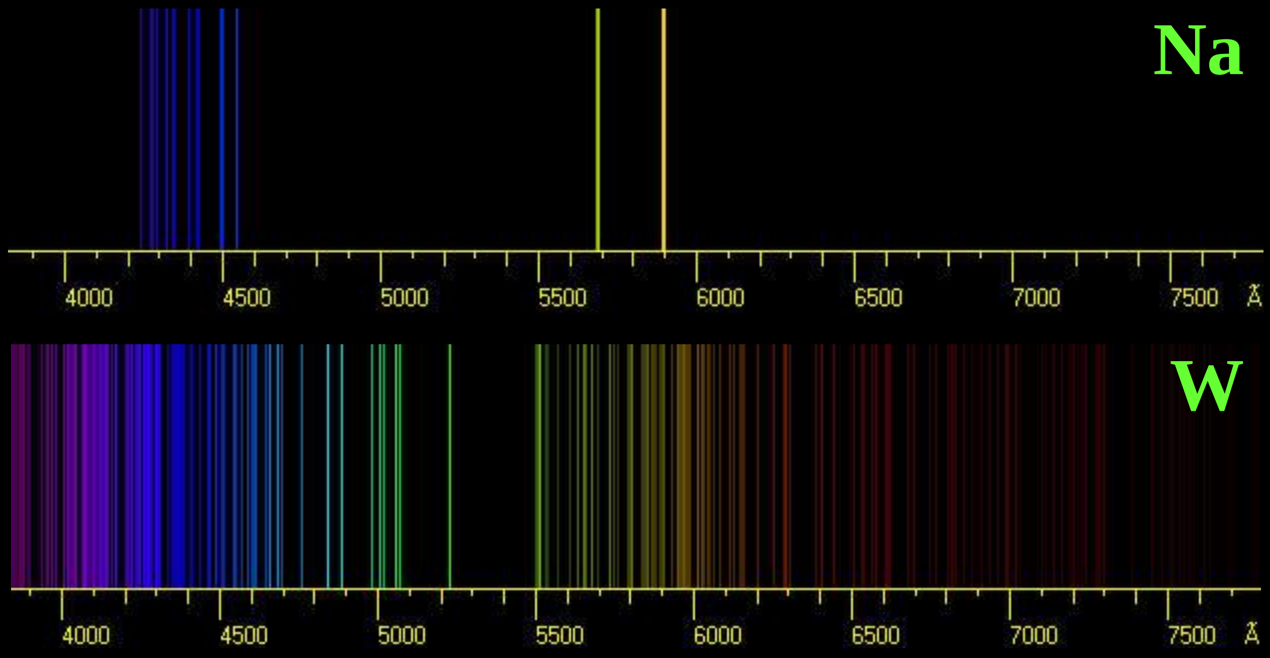
Emission Spectra

Determines Observed Colors Of lights & flames



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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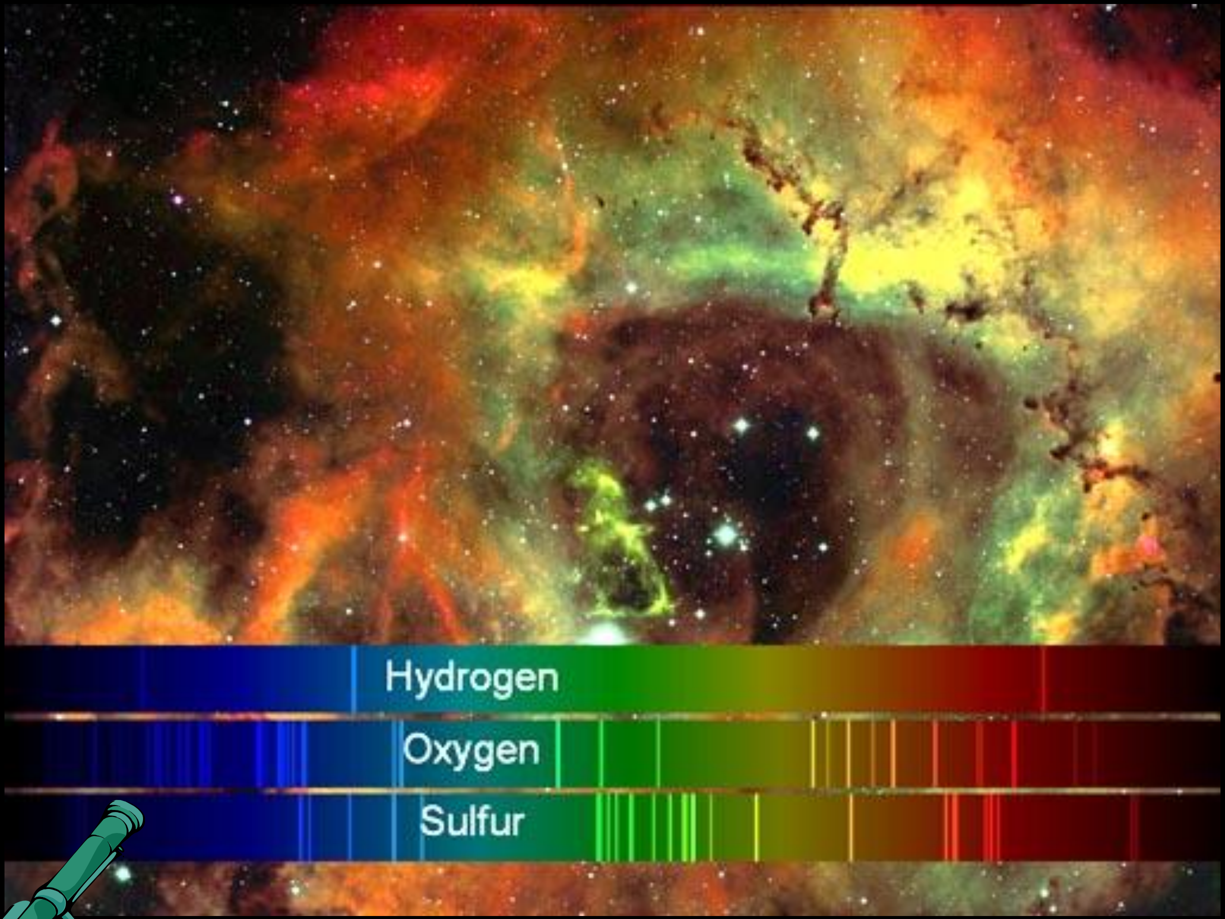
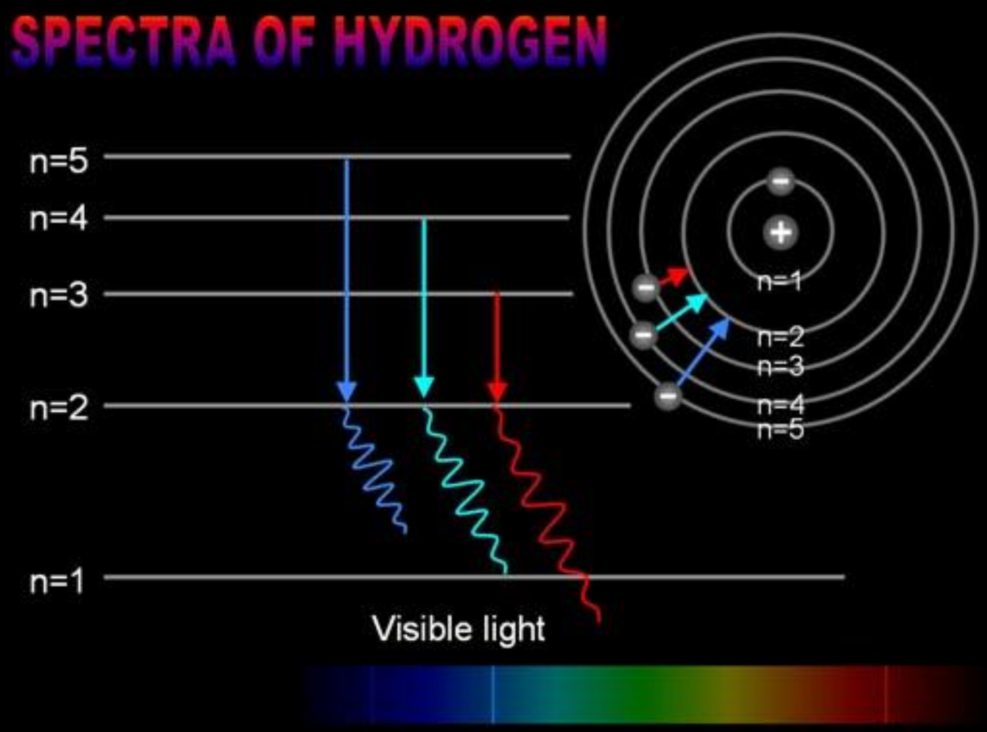
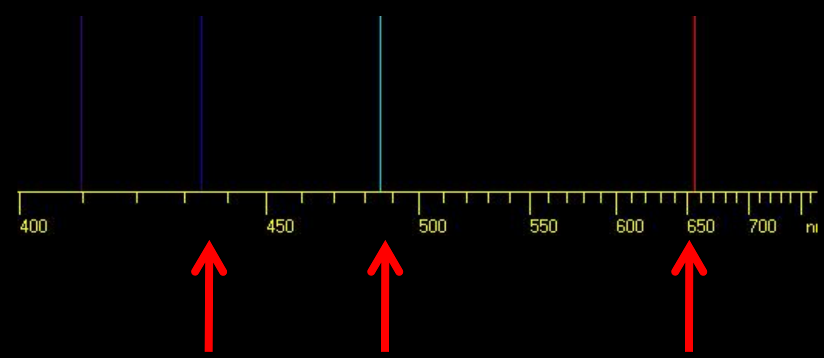
Emission Spectra: Astronomical Tool for Discovery



Presence of Hydrogen and Oxygen Exciting

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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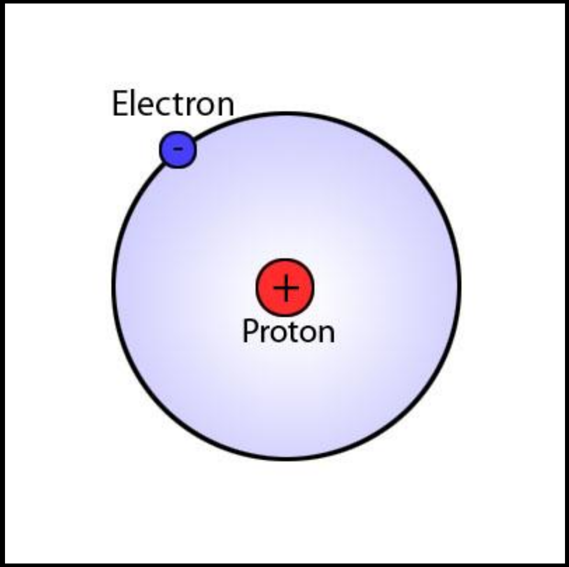
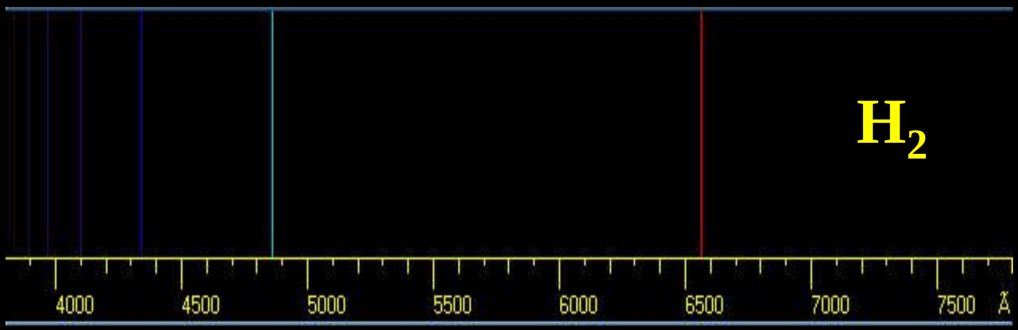
Bohr Model of the Hydrogen Atom

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



H_2

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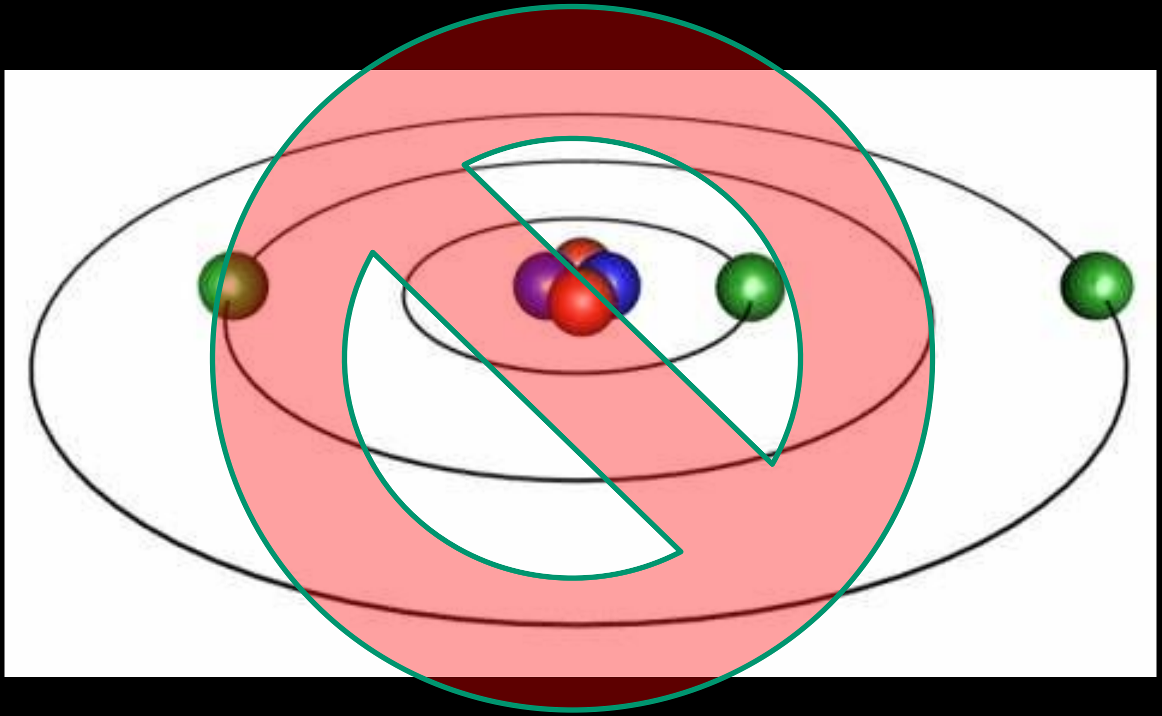
Heisenberg Uncertainty Principle

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)

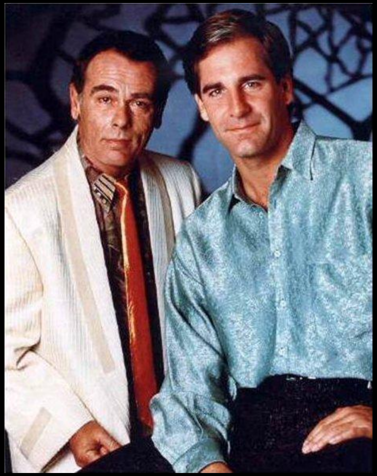
Wave-Particle Duality

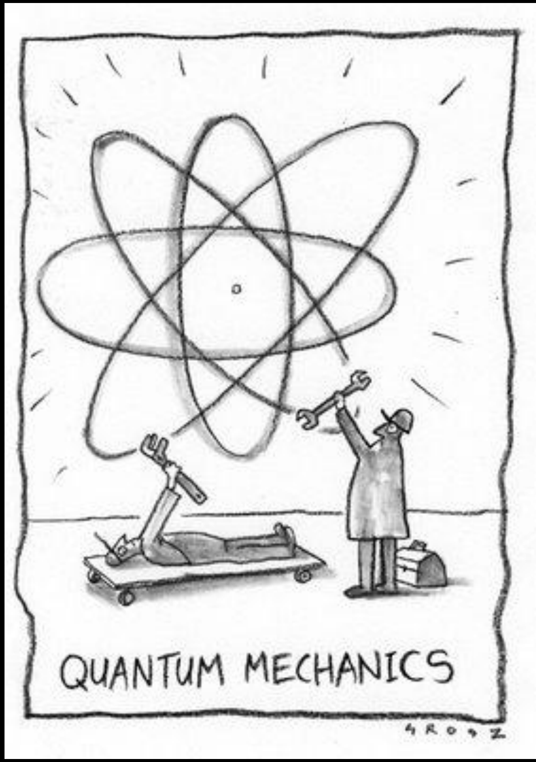
Explaining light and sub-atomic particles requires duality

Quantum Mechanics

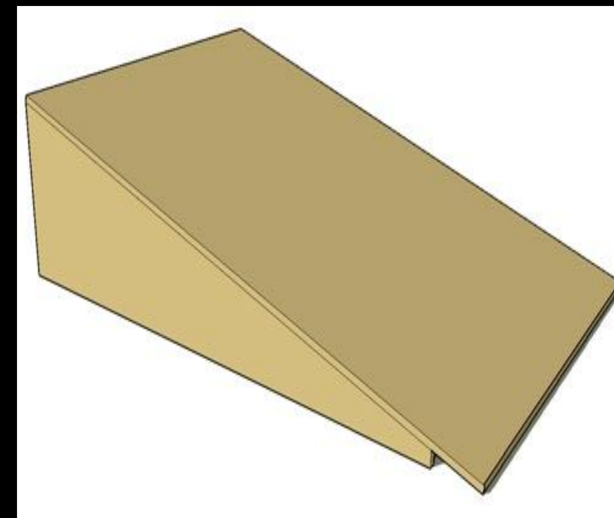
Discrete, non-continuous values of energy

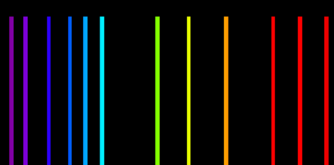
Energy "Leaps" from one level to another





Quantum Means “In Discrete Steps”





Quantized Process

Continuous Process

Quantum Mechanics

Schrödinger (1925) Wave Equation

$$H \Psi = E \Psi$$

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)

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

Ψ^2 Plot

Each electron: separate equation

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

Metalloids	Metals
Alkali Earth Metals	Halogens
Transition Metals	Noble Gases
Non Metals	Transactinides
Alkali Metals	Lanthanides
Actinides	

atomic number
symbol
atomic weight

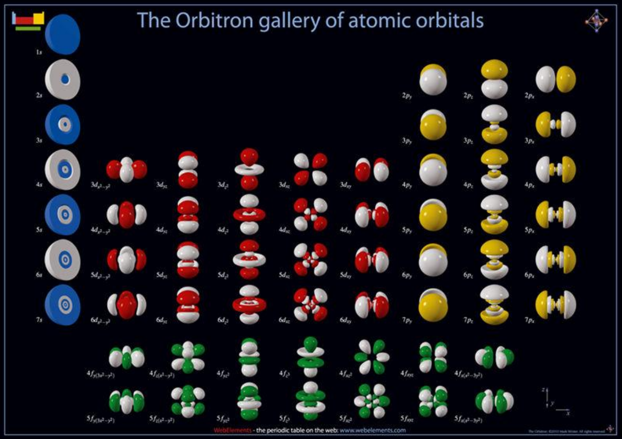
Element:

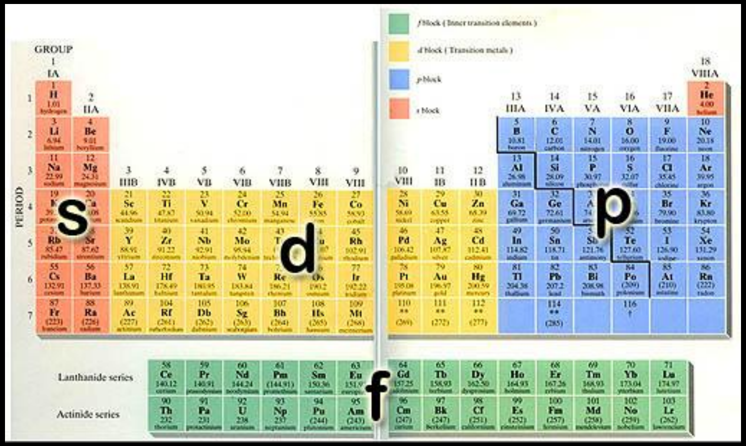
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	
1	1 H 1.01																	2 He 4	1
2	3 Li 6.94	4 Be 9.01											5 B 10.8	6 C 12	7 N 14	8 O 16	9 F 19	10 Ne 20.2	2
3	11 Na 23	12 Mg 24.3											13 Al 27	14 Si 28.1	15 P 31	16 S 32.1	17 Cl 35.5	18 Ar 39.9	3
4	19 K 39.1	20 Ca 40.1	21 Sc 45	22 Ti 47.9	23 V 50.9	24 Cr 52	25 Mn 54.9	26 Fe 55.8	27 Co 58.9	28 Ni 58.7	29 Cu 63.5	30 Zn 65.4	31 Ga 69.7	32 Ge 72.6	33 As 74.9	34 Se 79	35 Br 79.9	36 Kr 83.8	4
5	37 Rb 85.5	38 Sr 87.6	39 Y 88.9	40 Zr 91.2	41 Nb 92.9	42 Mo 95.9	43 Tc 98	44 Ru 101	45 Rh 103	46 Pd 106	47 Ag 108	48 Cd 112	49 In 115	50 Sn 119	51 Sb 122	52 Te 128	53 I 127	54 Xe 131	5
6	55 Cs 133	56 Ba 137	57 La 139	72 Hf 178	73 Ta 181	74 W 184	75 Re 186	76 Os 190	77 Ir 192	78 Pt 195	79 Au 197	80 Hg 201	81 Tl 204	82 Pb 207	83 Bi 209	84 Po 209	85 At 210	86 Rn 222	6
7	87 Fr 223	88 Ra 226	89 Ac 227	104 Rf 261	105 Db 262	106 Sg 266	107 Bh 264	108 Hs 269	109 Mt 268	110 Ds 281	111 Rg 272	112 Uub 285	113 Uut 284	114 Uuq 289	115 Uup 288	116 Uuh 292	117 Uus	118 Uuo	7

Lanthanide Series	6	58 Ce 140	59 Pr 141	60 Nd 144	61 Pm 145	62 Sm 150	63 Eu 152	64 Gd 157	65 Tb 159	66 Dy 162	67 Ho 165	68 Er 167	69 Tm 169	70 Yb 173	71 Lu 175
Actinide Series	7	90 Th 232	91 Pa 231	92 U 238	93 Np 237	94 Pu 244	95 Am 243	96 Cm 247	97 Bk 247	98 Cf 251	99 Es 252	100 Fm 257	101 Md 258	102 No 259	103 Lr 262

Quantum Numbers

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





Principle Quantum Number (n)

Value of n = 1, 2, 3, …, ∞

Represents average energy of electron orbital

Increasing n → increasing energy

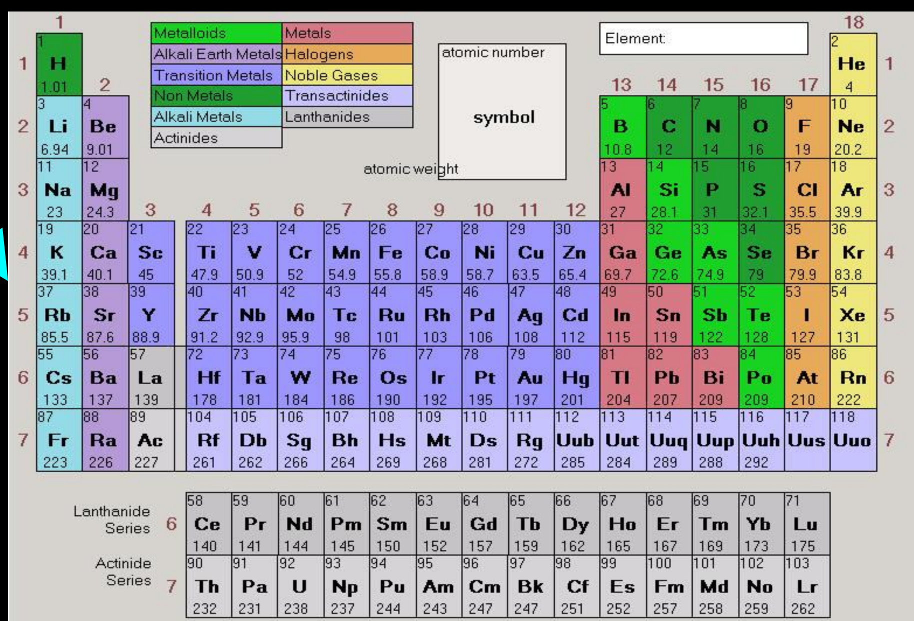
Increasing n → increasing distance from the nucleus

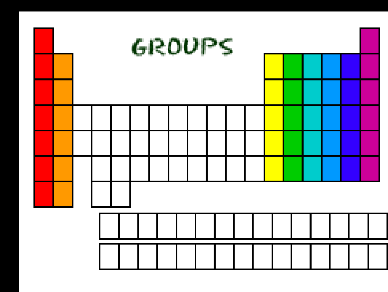
Corresponds to the n value (row) on the periodic table

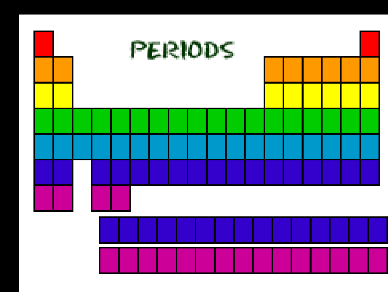
Corresponds to number of sub-orbitals available

Maximum number of electrons per n = $2n^2$

n







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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"

s p d

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 $\ell = 4\ell + 2$

Magnetic Quantum Number (m_ℓ)

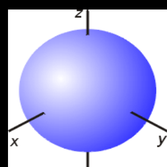
Value of $-\ell \leq m_l \leq \ell$

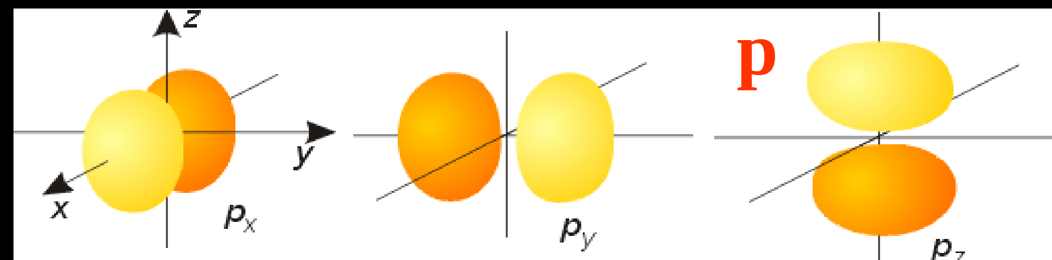
Represents spatial orientation (with respect to external field)

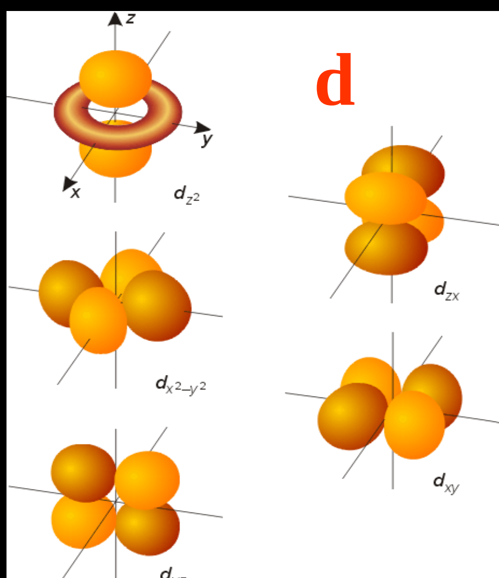
Corresponds to probability of finding electron

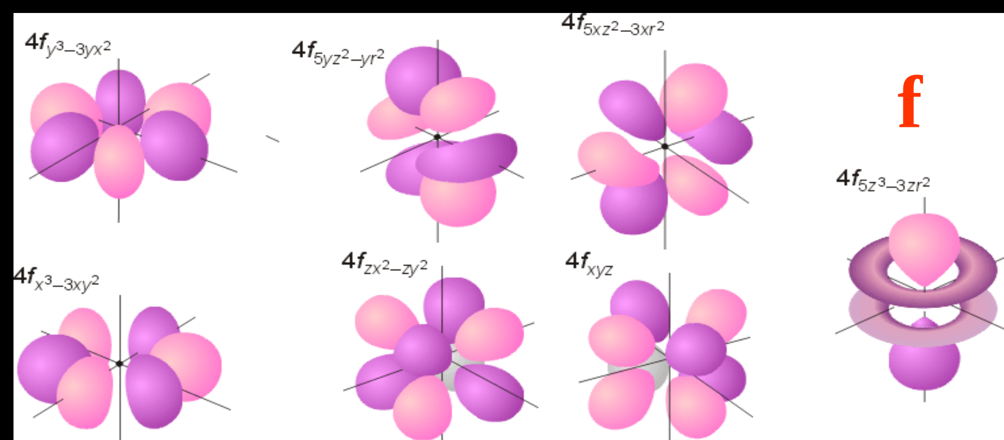
Each orbital (ℓ) has separate (magnetic) quantum number (s)

s



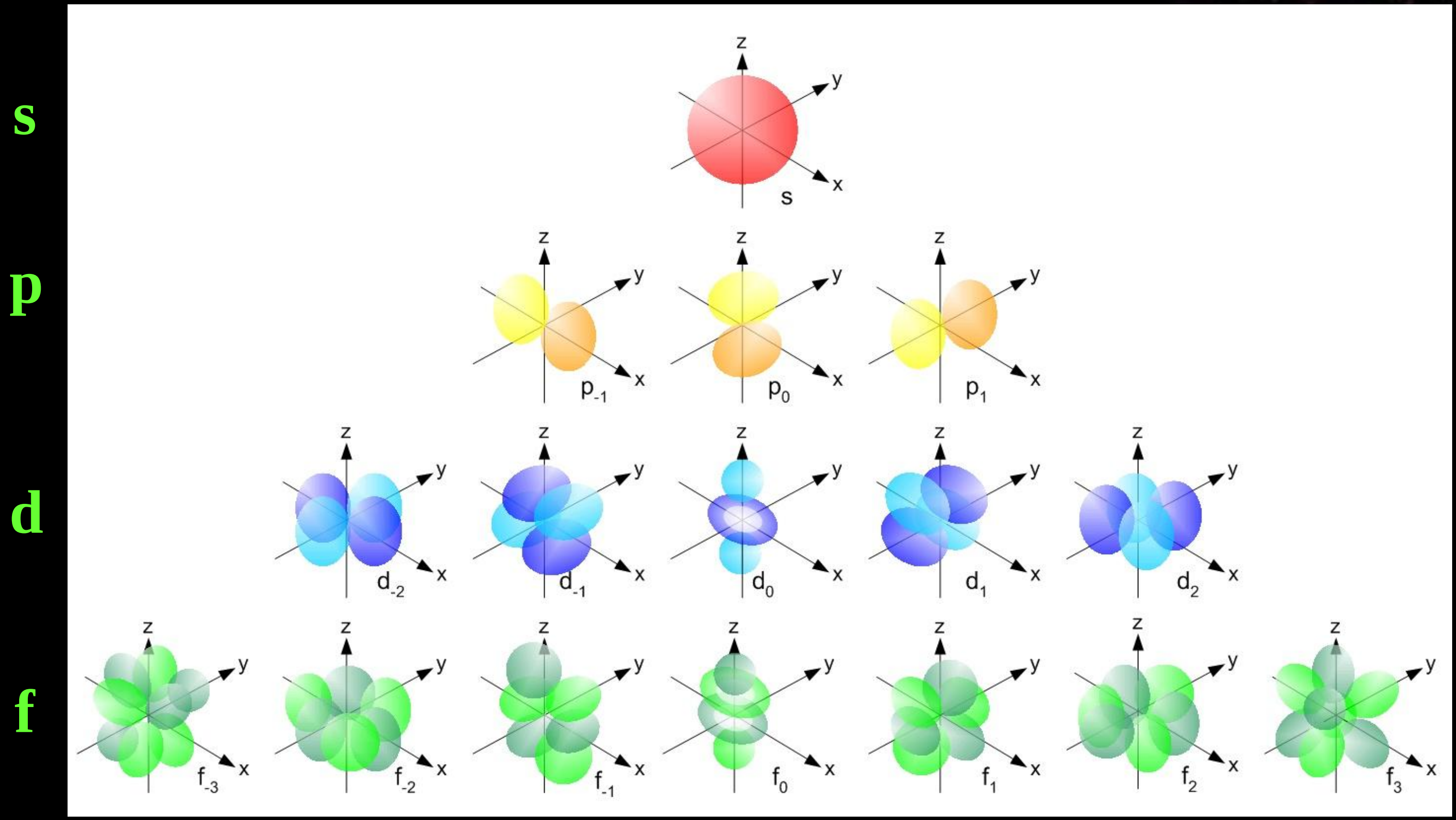






LPT

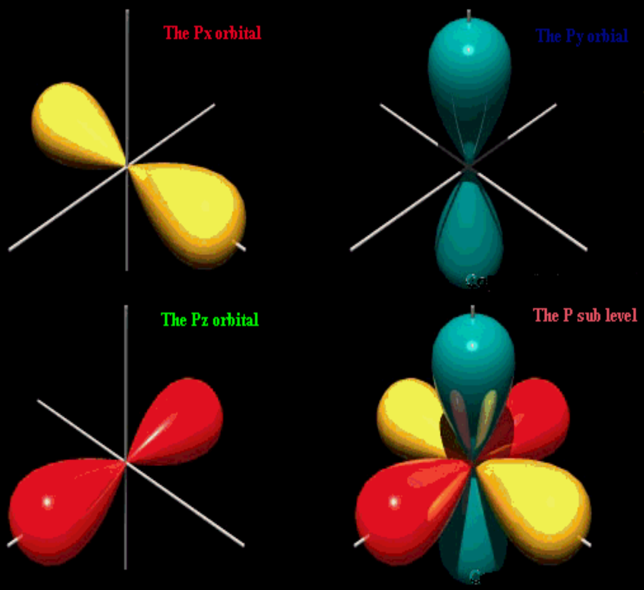
Planets Travel in Orbits
Electrons Occupy Orbitals



LPT

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

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

LPT

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)

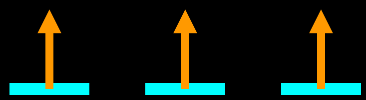
Hund's Rule

Based on observations of spectral energy

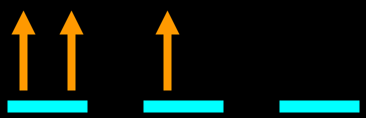
Each orbital gets one electron before accepting a second

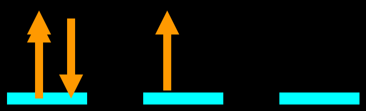
Orbitals will fill with maximum number of unpaired electrons

For P Orbitals



Never





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

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

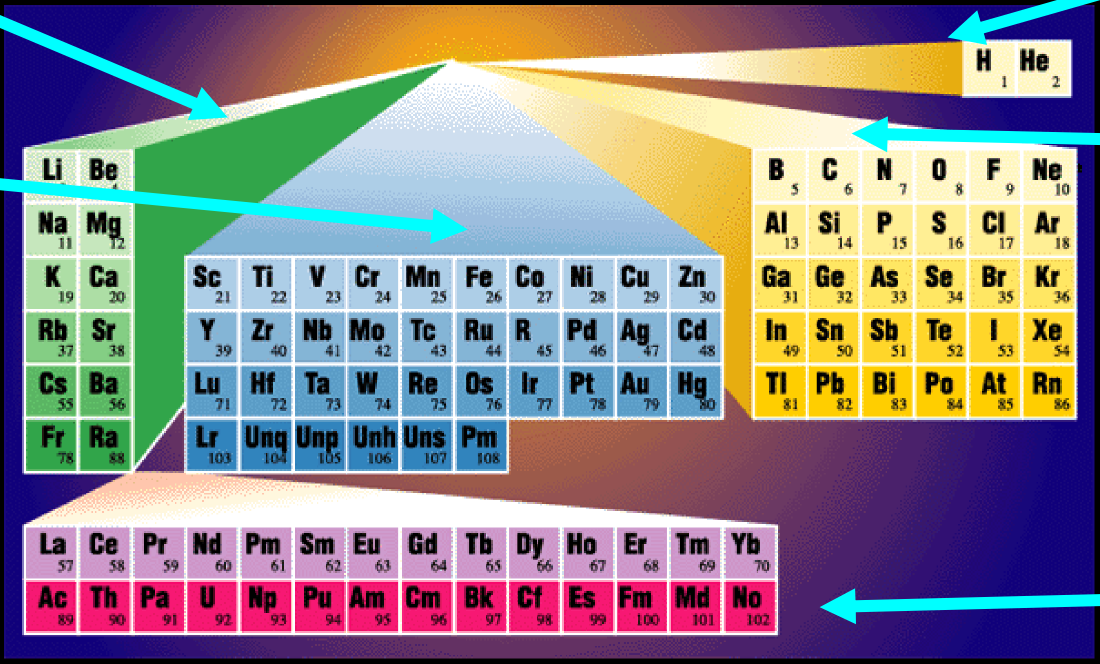
s
2 spaces

d
10 spaces

1 s
2 spaces

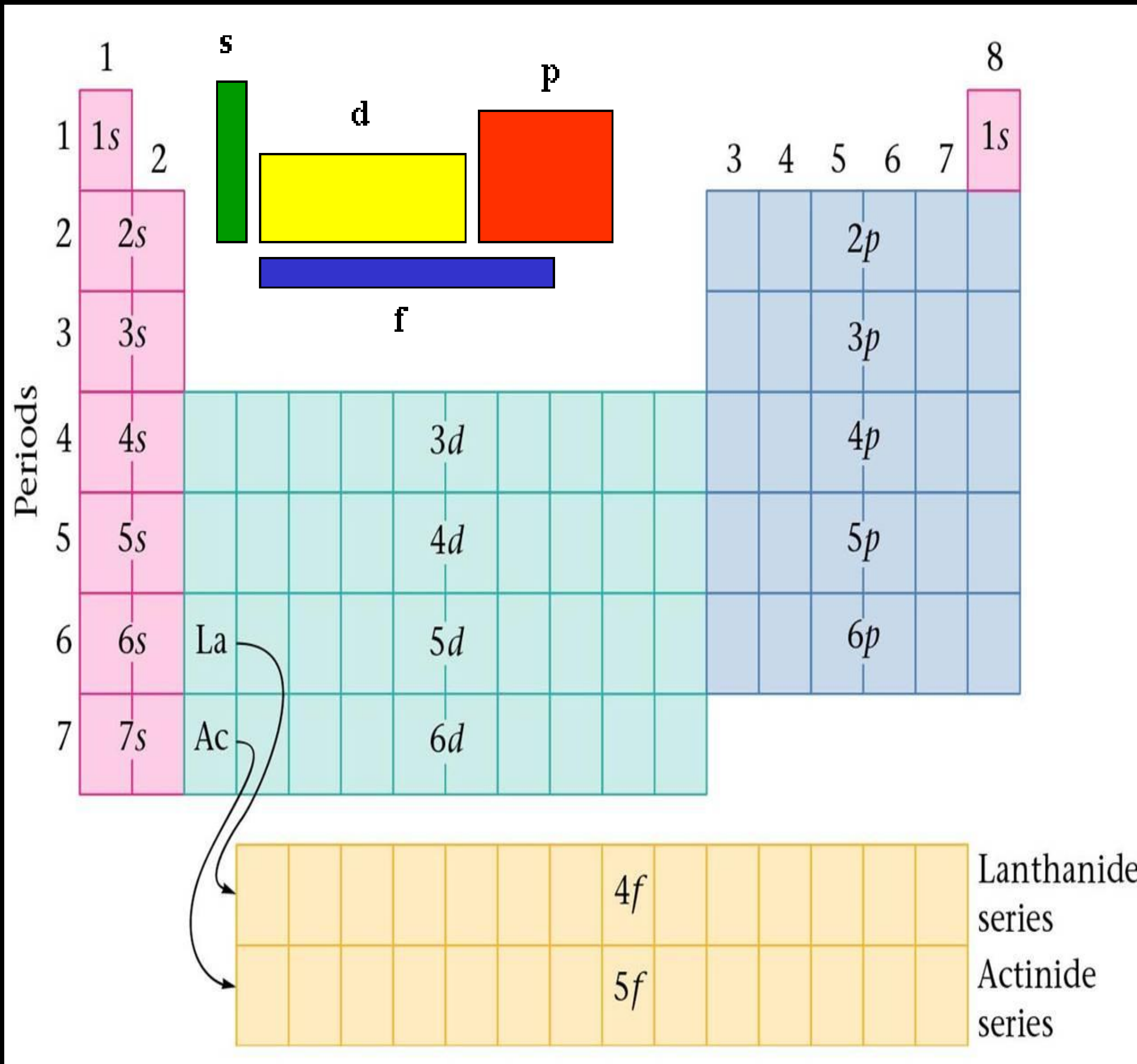
p
6 spaces

f
14 spaces

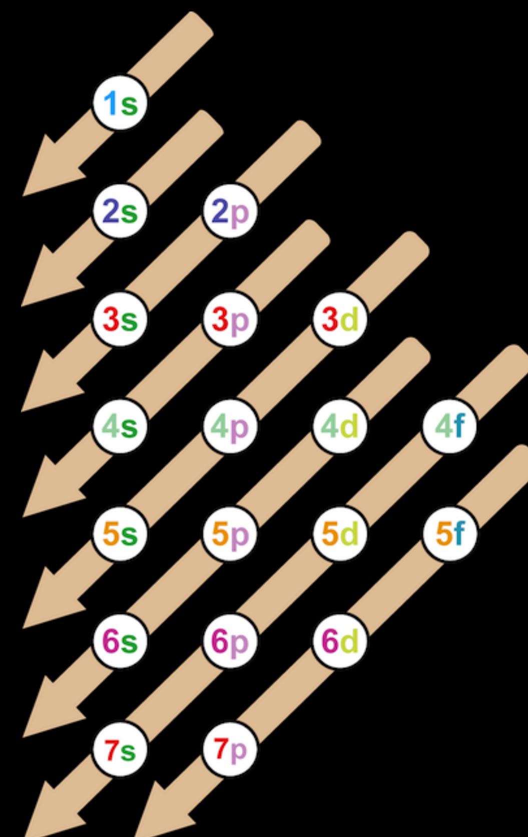


LPT

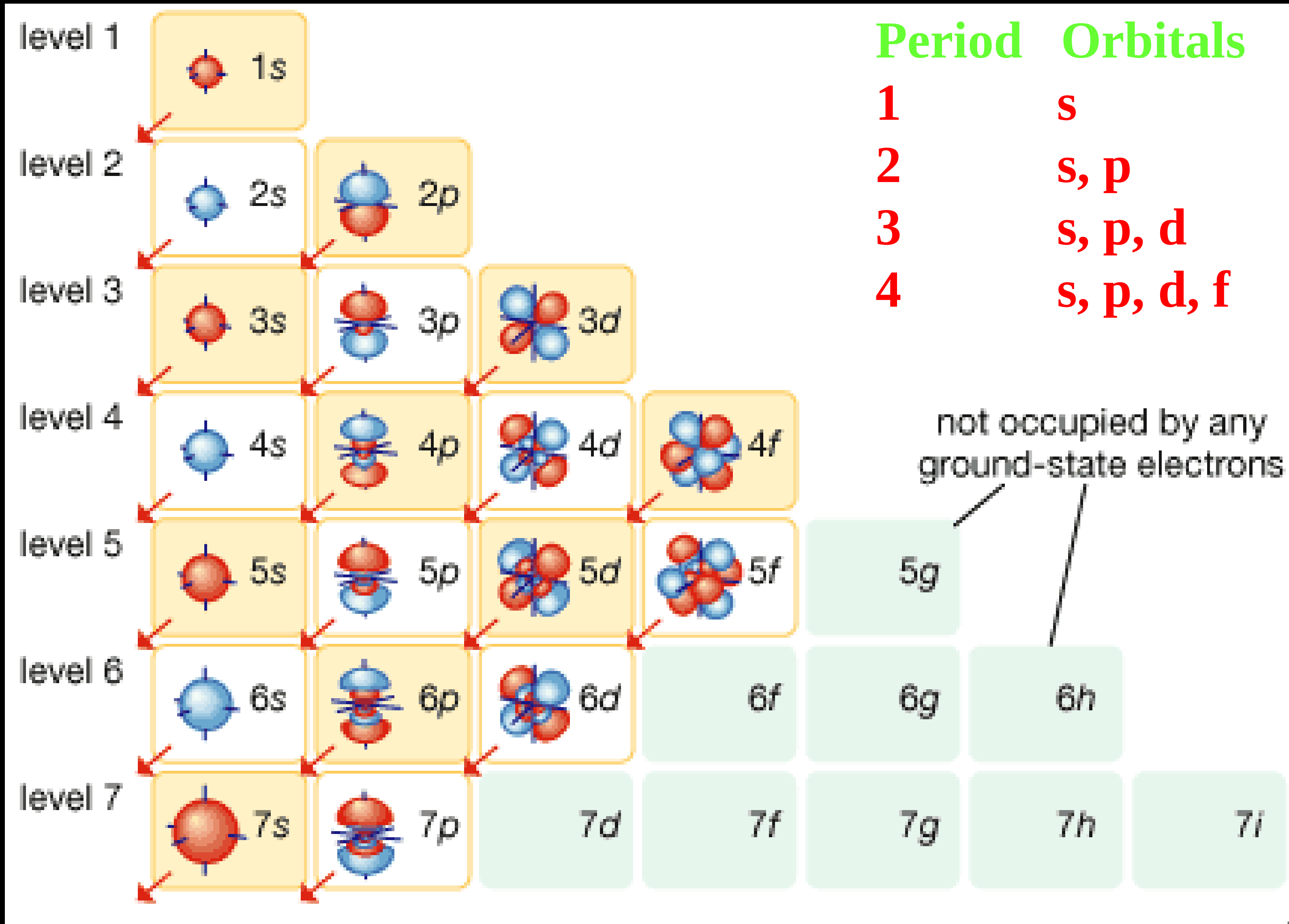
Orbital Filling



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

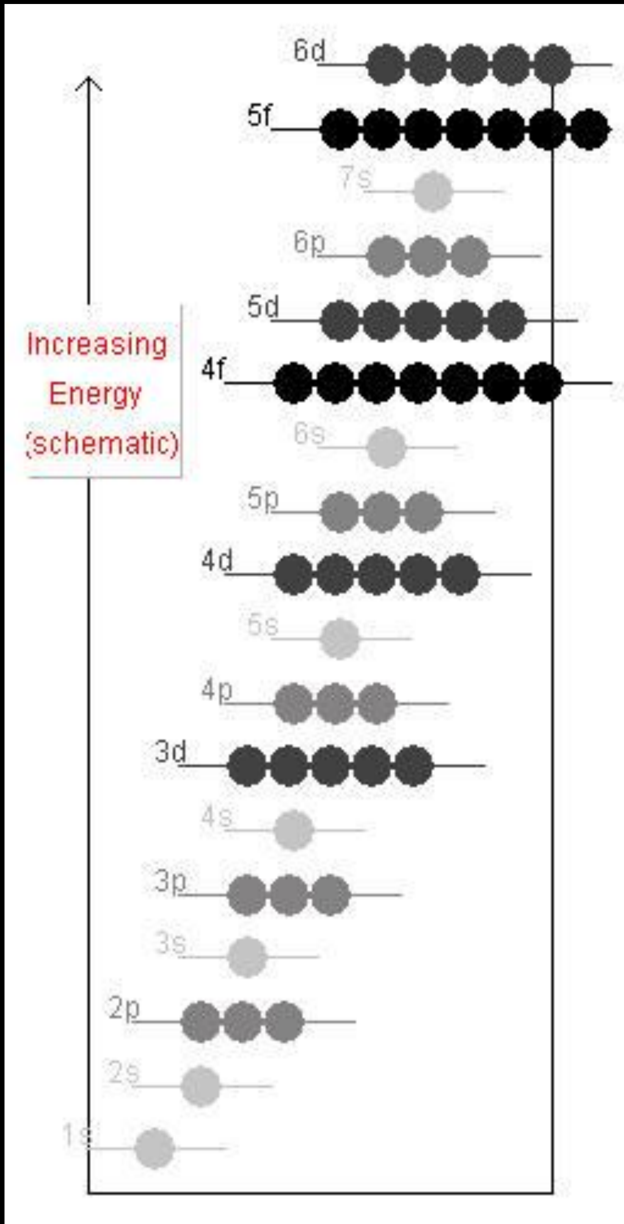


Available Orbitals

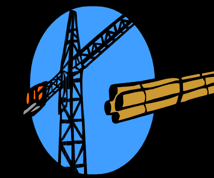


Period	Orbitals
1	s
2	s, p
3	s, p, d
4	s, p, d, f

LPT



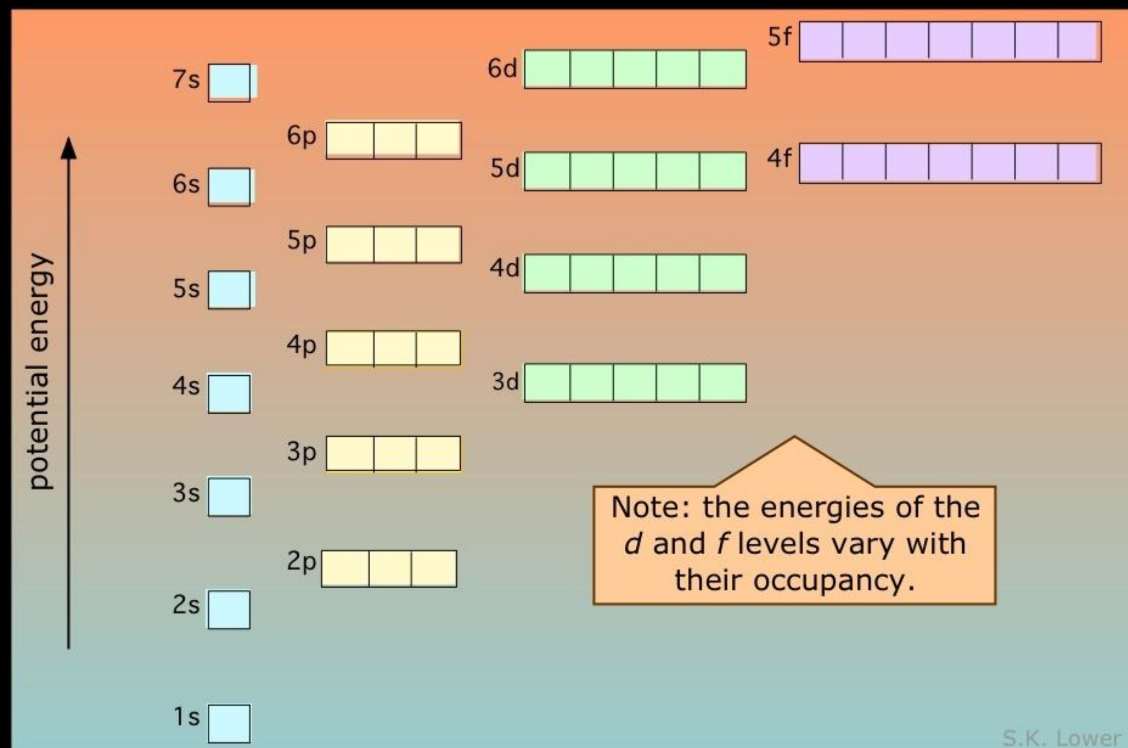
Aufbau Principle



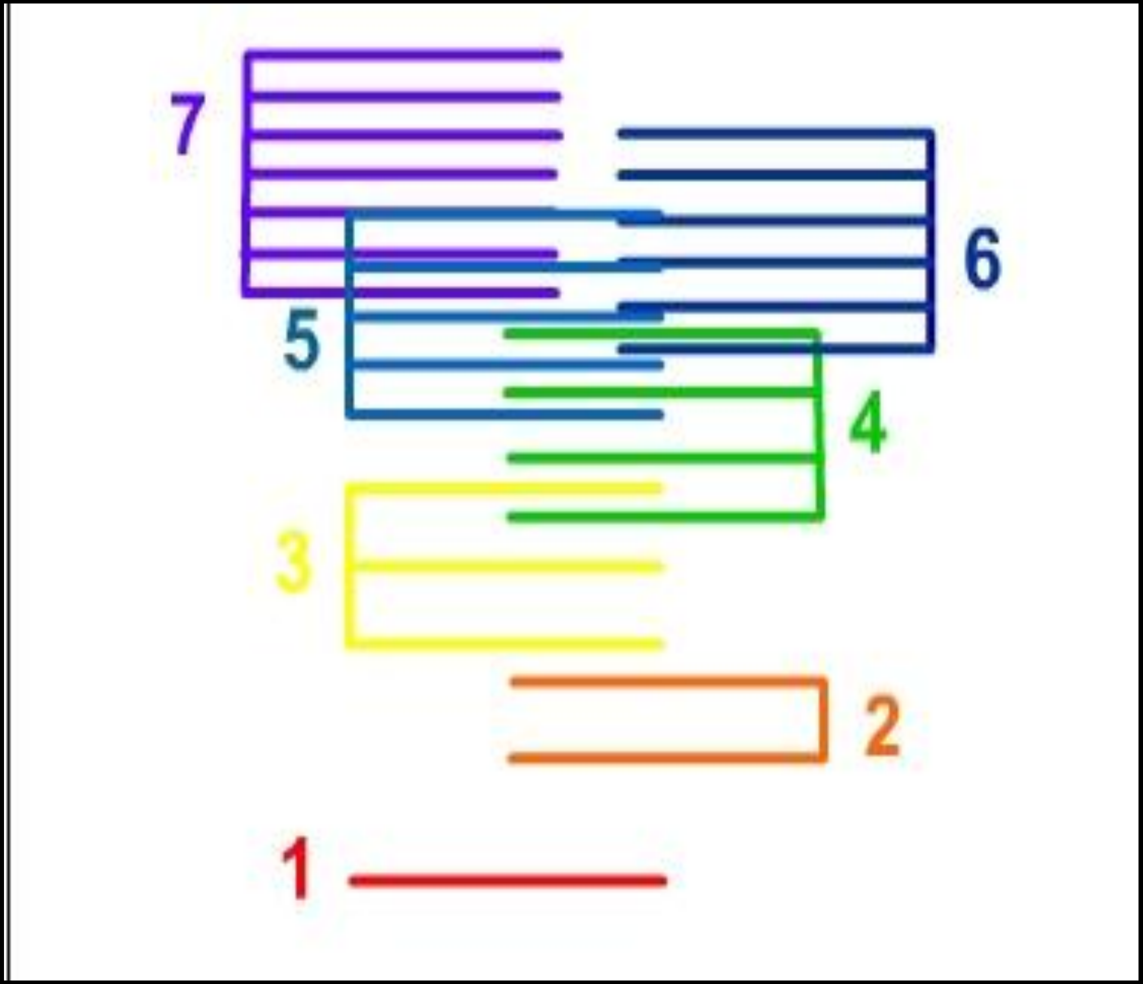
German for "construction" or build-up

Termed coined by Niels Bohr in 1920

Electron Configurations constructed by progressively adding electrons

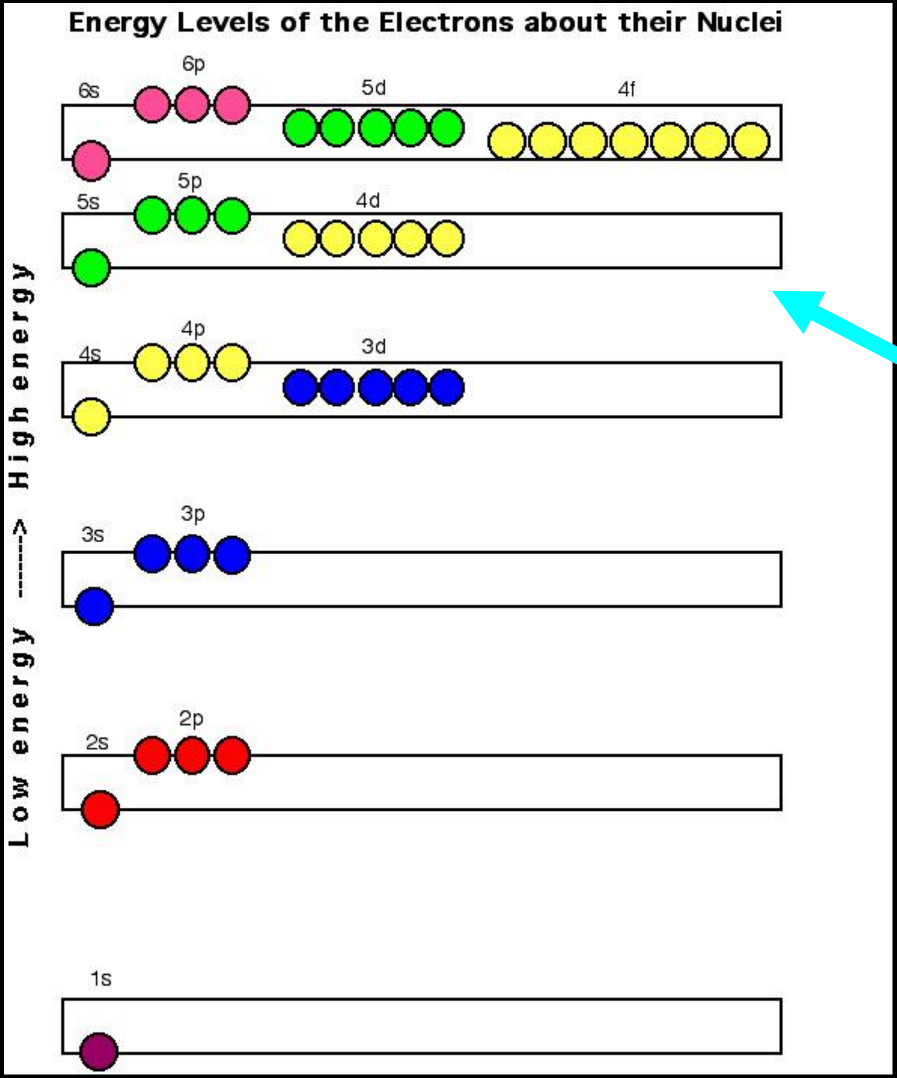


The Orbital Energies Overlap
Explains Transition Metal Valence Variability



LPT

Electron Energy Diagram

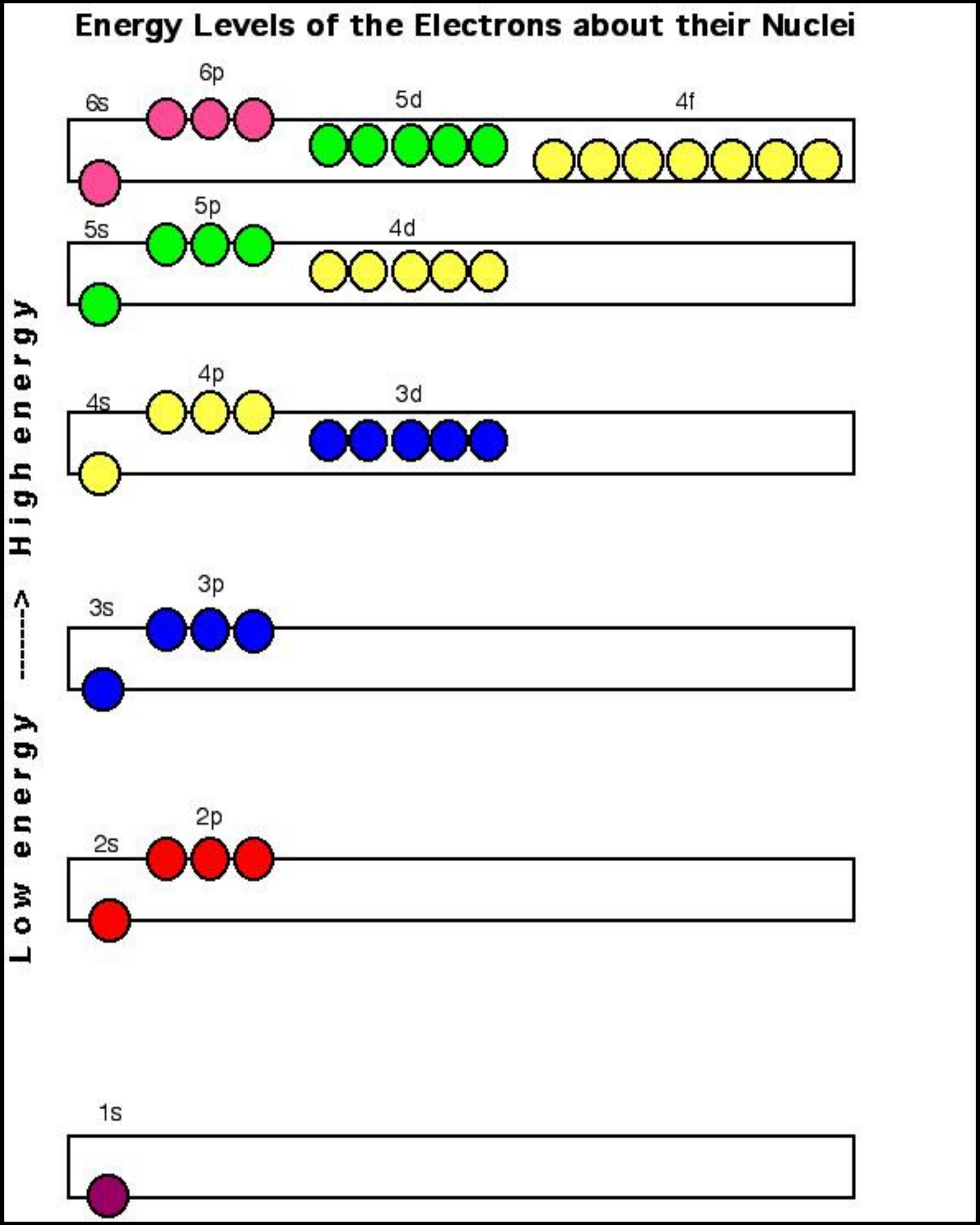


Energies

Large Between n's
Small Between ℓ's

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

LPT



Worksheet

Start at lower level

Add electrons
Until correct # reached

2 electrons per orbital

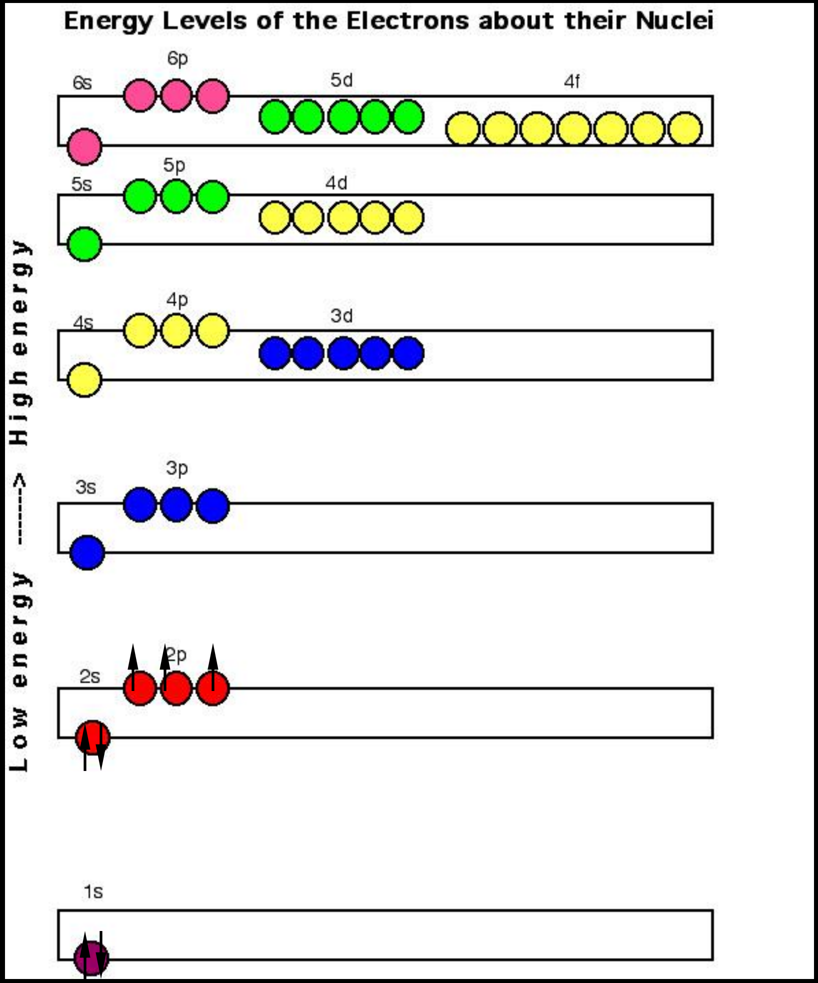
This corresponds to
Periodic Table
Arrangement of Elements

LPT

Worksheet - Examples

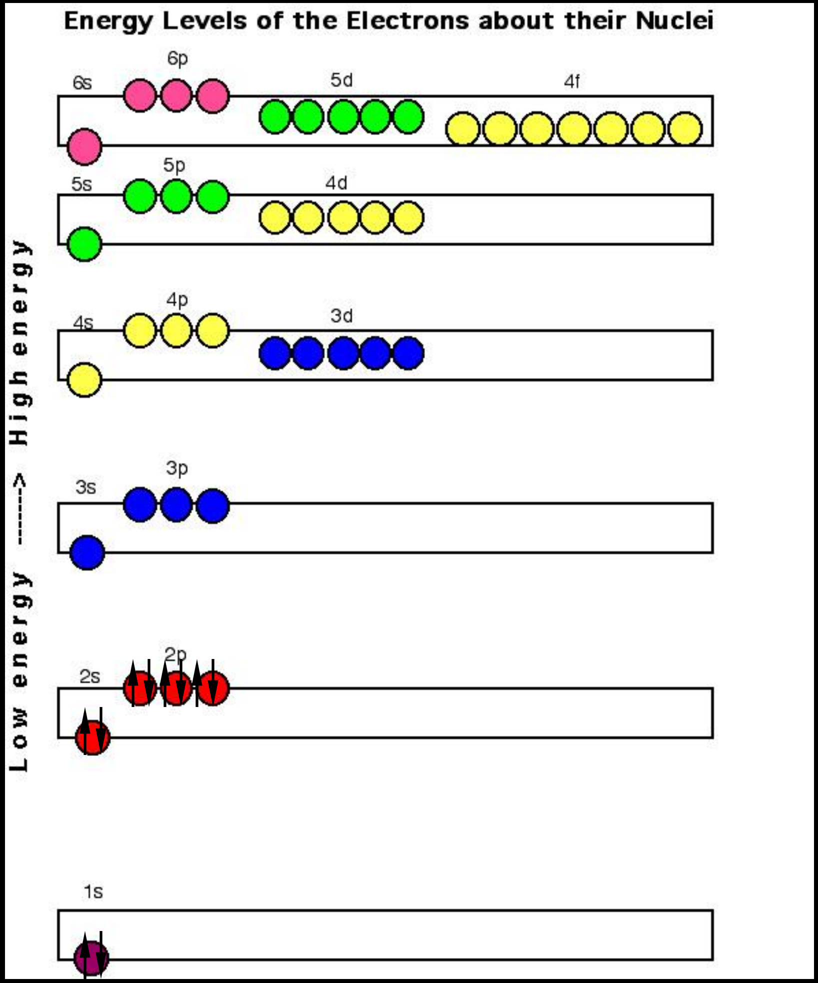
For Nitrogen (Z= 7)

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



For Neon (Z= 10)

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



Electron Configuration Nomenclature

Shows sub-shell (orbital) distribution of electrons

# of electrons in orbital

Energy Level (n)

$3\,s^{2}$

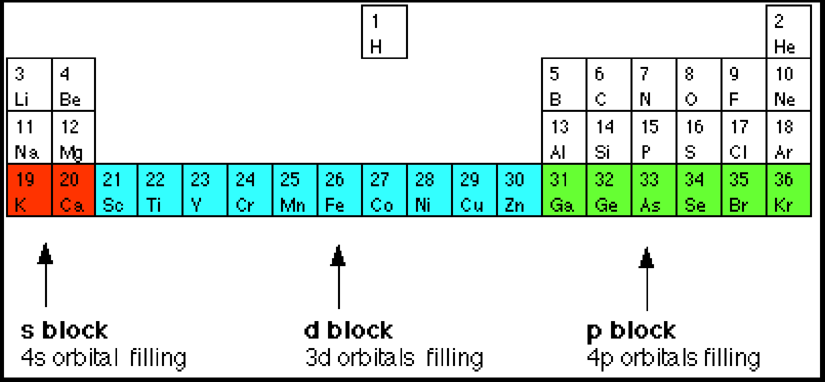
Orbital type

Use Periodic Table to list electrons

List electron configuration in order of atomic number

Start with H (Z=1)

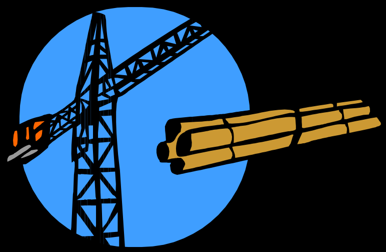
Continue adding electrons until desired element is reached



LPT

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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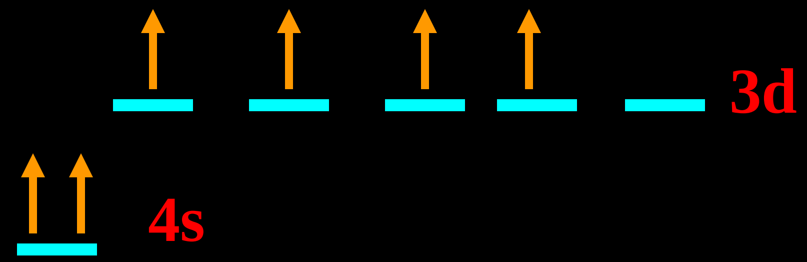
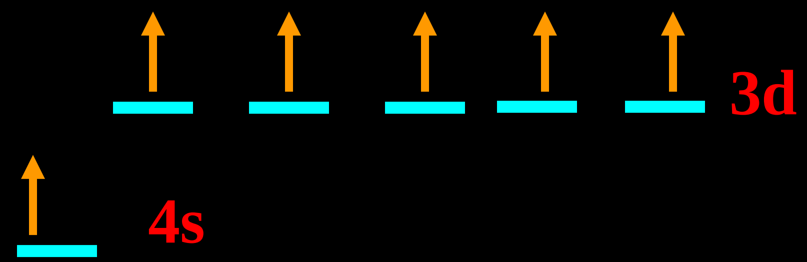
Aufbau Exceptions

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

Electron Pairing Affects Magnetic Properties

Paramagnetic elements

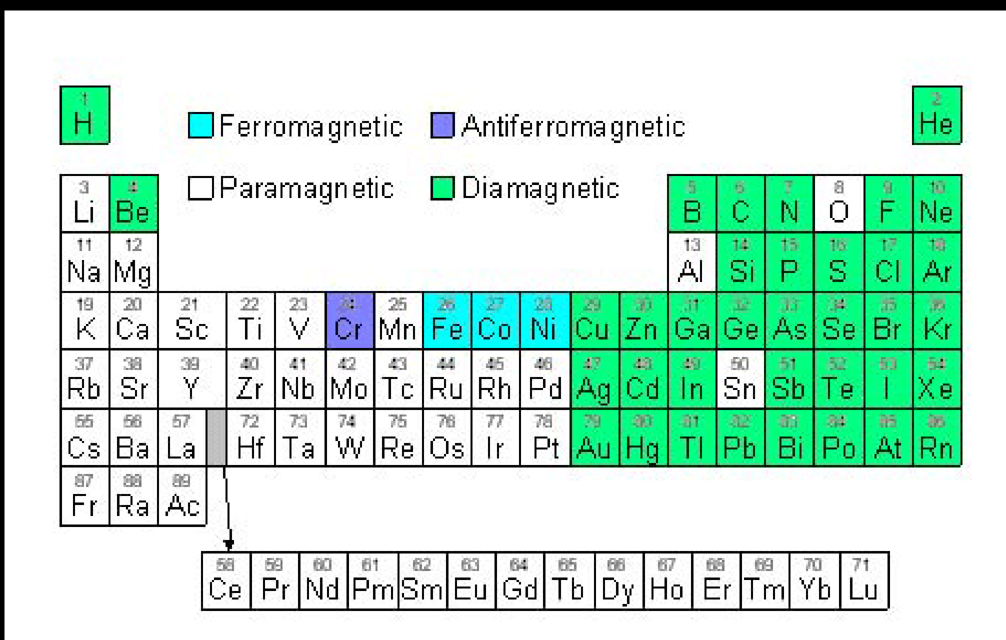
Unpaired electrons attracted to magnetic fields

Diamagnetic elements

Paired electrons slightly repelled by magnetic fields

Ferromagnetic

Elements having very high magnetic properties



Magnitude affected by:

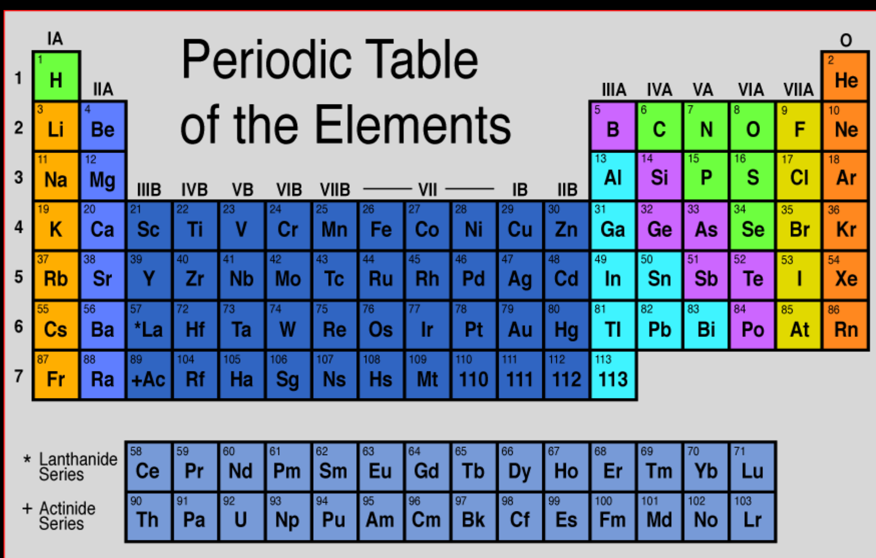
Magnetic field strength

Temperature

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

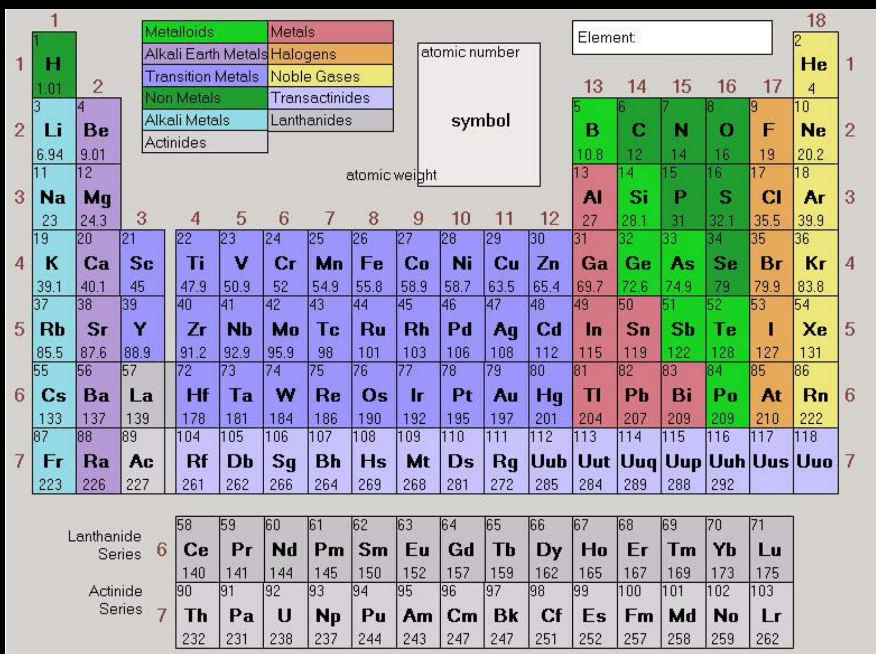
Highest energy level (Outer-most shell)

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 $1s^2 2s^2 2p^6 3s^1$

Na^+ $1s^2 2s^2 2p^6$

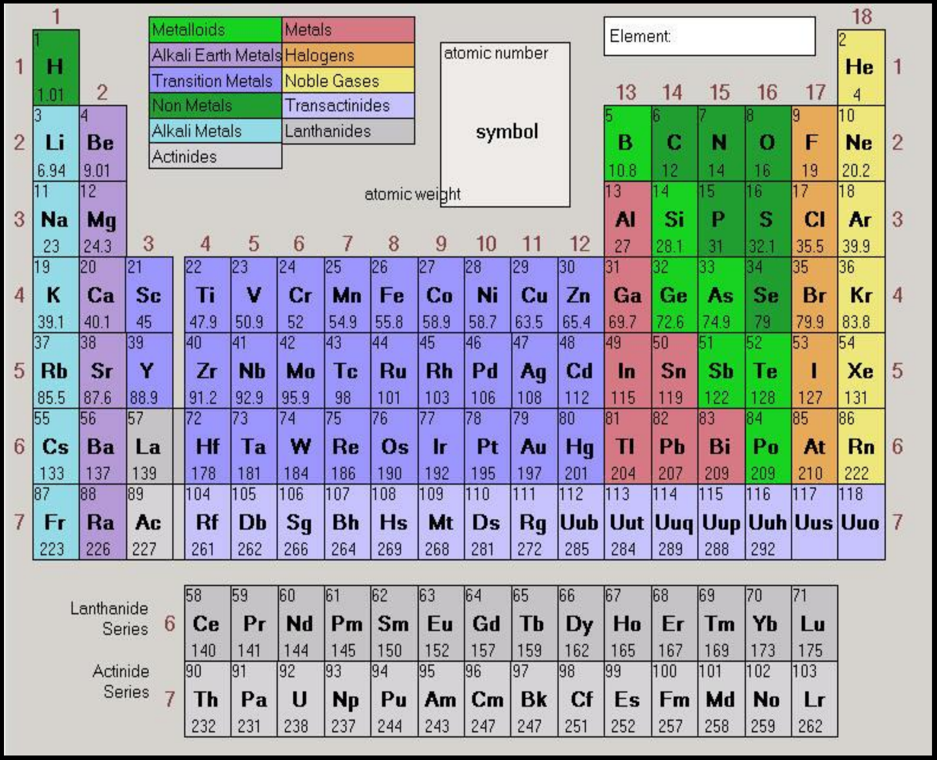
Ne $1s^2 2s^2 2p^6$

Isoelectronic

O $1s^2 2s^2 2p^4$

O^{2-} $1s^2 2s^2 2p^6$

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



Atoms gain or lose electrons

To acquire a noble configuration

LPT

Isoelectronic Atoms

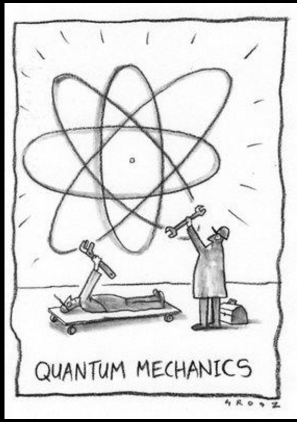
Any pair of atoms with the same electronic configuration is isoelectronic

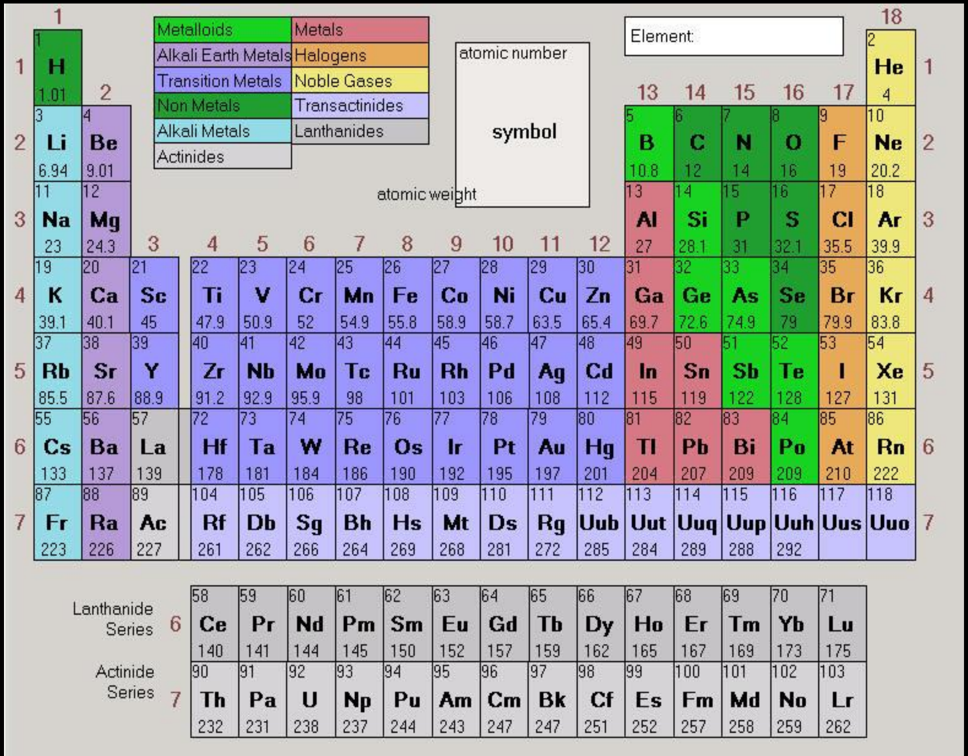
Ne, F^-, O^{2-} are isoelectronic

Ar, Cl^-, S^{2-} are isoelectronic

Mg^{2+} , Na^+ , Ne are isoelectronic

Ca^{2+} , K^+ , Ar are isoelectronic



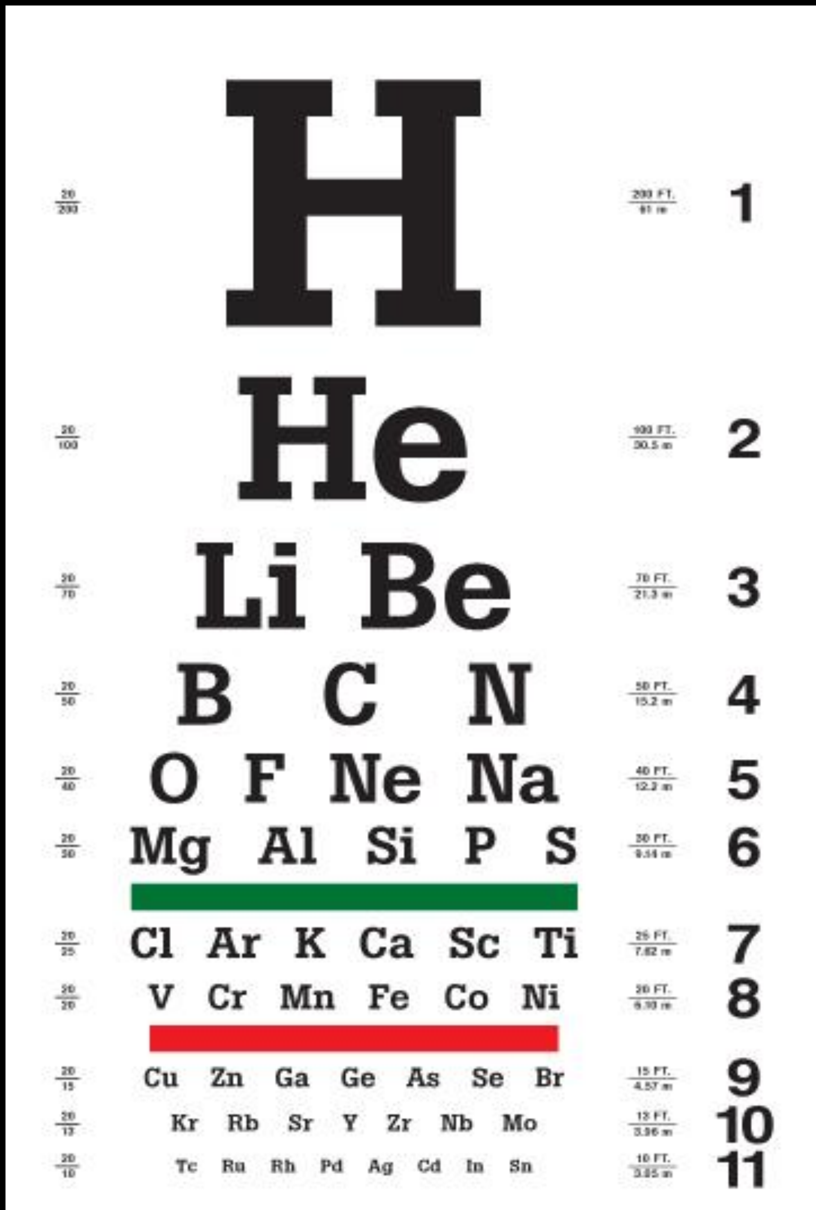


Metalloids	Metals
Alkali Earth Metals	Halogens
Transition Metals	Noble Gases
Non Metals	Transactinides
Alkali Metals	Lanthanides
Actinides	

Element: atomic number / symbol / atomic weight

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	
1	1 H 1.01																	2 He 4	1
2	3 Li 6.94	4 Be 9.01											5 B 10.8	6 C 12	7 N 14	8 O 16	9 F 19	10 Ne 20.2	2
3	11 Na 23	12 Mg 24.3											13 Al 27	14 Si 28.1	15 P 31	16 S 32.1	17 Cl 35.5	18 Ar 39.9	3
4	19 K 39.1	20 Ca 40.1	21 Sc 45	22 Ti 47.9	23 V 50.9	24 Cr 52	25 Mn 54.9	26 Fe 55.8	27 Co 58.9	28 Ni 58.7	29 Cu 63.5	30 Zn 65.4	31 Ga 69.7	32 Ge 72.6	33 As 74.9	34 Se 79	35 Br 79.9	36 Kr 83.8	4
5	37 Rb 85.5	38 Sr 87.6	39 Y 88.9	40 Zr 91.2	41 Nb 92.9	42 Mo 95.9	43 Tc 98	44 Ru 101	45 Rh 103	46 Pd 106	47 Ag 108	48 Cd 112	49 In 115	50 Sn 119	51 Sb 122	52 Te 128	53 I 127	54 Xe 131	5
6	55 Cs 133	56 Ba 137	57 La 139	72 Hf 178	73 Ta 181	74 W 184	75 Re 186	76 Os 190	77 Ir 192	78 Pt 195	79 Au 197	80 Hg 201	81 Tl 204	82 Pb 207	83 Bi 209	84 Po 209	85 At 210	86 Rn 222	6
7	87 Fr 223	88 Ra 226	89 Ac 227	104 Rf 261	105 Db 262	106 Sg 266	107 Bh 264	108 Hs 269	109 Mt 268	110 Ds 281	111 Rg 272	112 Uub 285	113 Uut 284	114 Uuq 289	115 Uup 288	116 Uuh 292	117 Uus	118 Uuo	7

Lanthanide Series	6	58 Ce 140	59 Pr 141	60 Nd 144	61 Pm 145	62 Sm 150	63 Eu 152	64 Gd 157	65 Tb 159	66 Dy 162	67 Ho 165	68 Er 167	69 Tm 169	70 Yb 173	71 Lu 175
Actinide Series	7	90 Th 232	91 Pa 231	92 U 238	93 Np 237	94 Pu 244	95 Am 243	96 Cm 247	97 Bk 247	98 Cf 251	99 Es 252	100 Fm 257	101 Md 258	102 No 259	103 Lr 262



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