

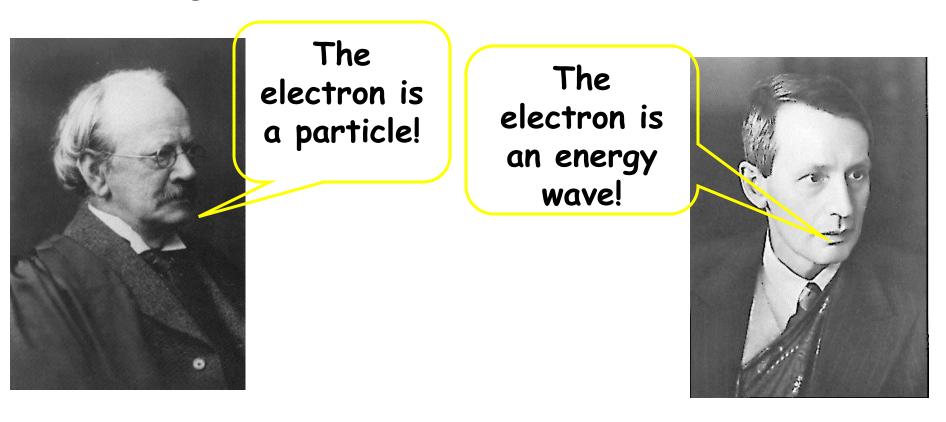
Quantum mechanics.

Cartoon courtesy of NearingZero.net

Wave-Particle Duality

JJ Thomson won the Nobel prize for describing the electron as a particle.

His son, George Thomson won the Nobel prize for describing the wave-like nature of the electron.



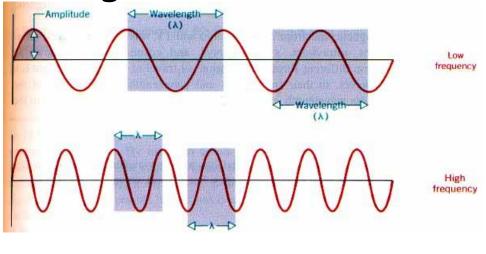
The Wave-like Electron



The electron propagates through space as an energy wave. To understand the atom, one must understand the behavior of electromagnetic waves.

Louis deBroglie

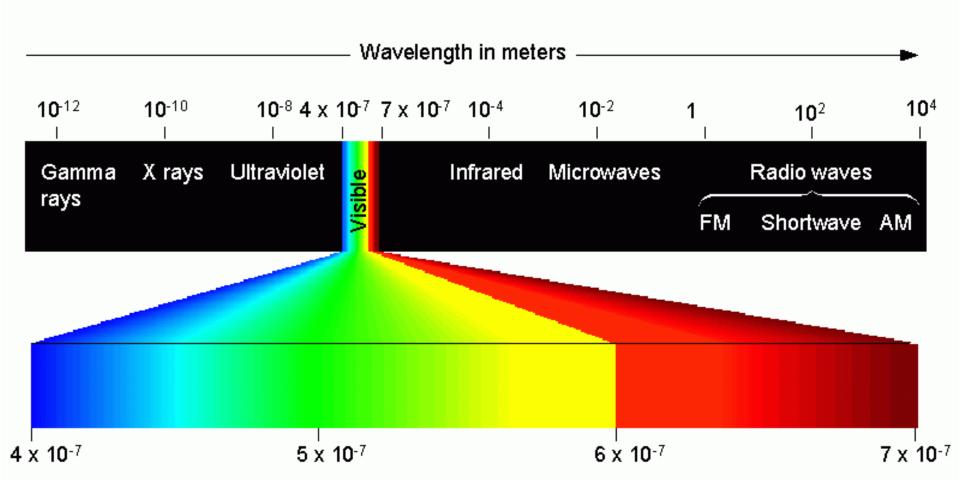
Electromagnetic radiation propagates through space as a wave moving at the speed of light.



$$c = v\lambda$$

C = speed of light, a constant (3.00 x 10⁸ m/s) v = frequency, in units of hertz (hz, sec⁻¹) λ = wavelength, in meters

Types of electromagnetic radiation:



Max Planck

- figured out that when a solid substance is heated, it gives off energy in "chunks"
- later called quantums of energy
 - quantum means fixed amount
- noticed that different substances released different "chunks" of energy



The energy (E) of electromagnetic radiation is directly proportional to the frequency (v) of the radiation.

E = hv

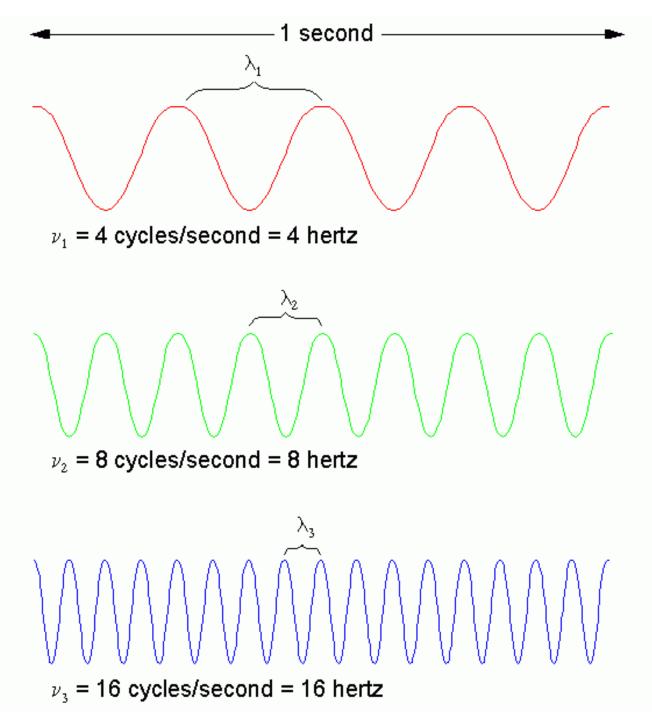
E = Energy, in units of Joules (kg \cdot m²/s²)

 $h = Planck's constant (6.626 \times 10-34 \text{ J} \cdot \text{s})$

v = frequency, in units of hertz (hz, sec⁻¹)

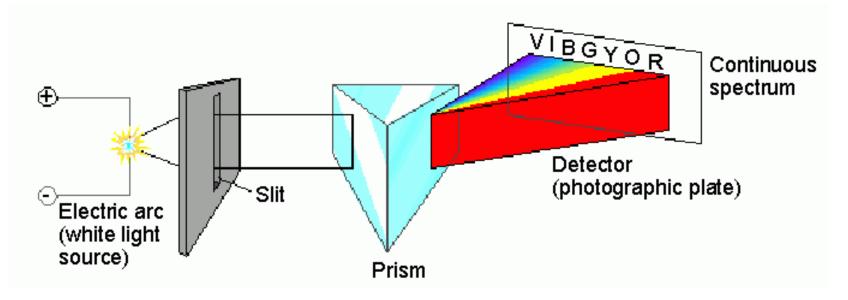
Long Wavelength = Low Frequency = Low ENERGY

Short Wavelength = High Frequency = High ENERGY



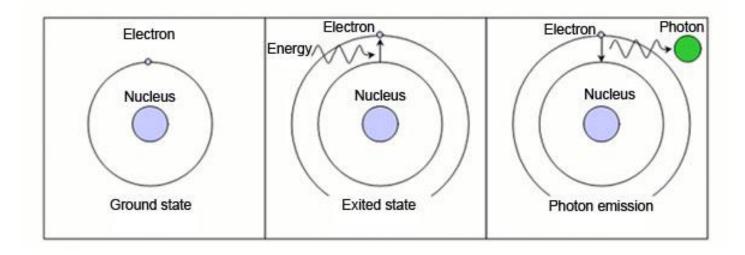
Spectroscopic analysis of the visible spectrum...

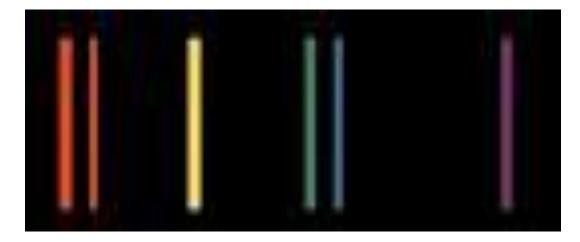
produces all of the colors in a continuous spectrum



How does matter produce light?

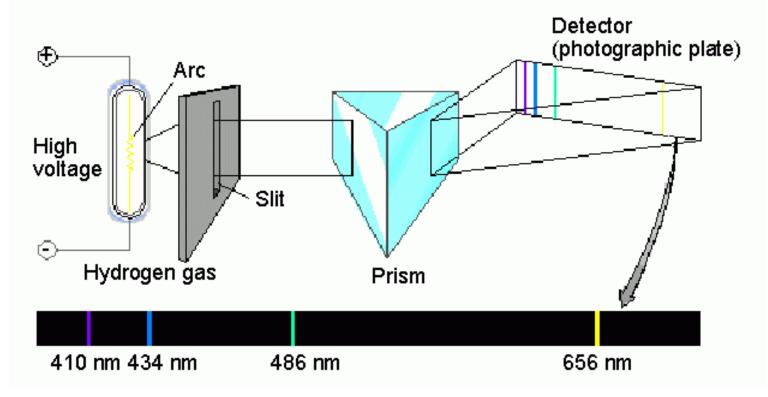
 When an electron in the ground state (lowest energy level that is natural) is promoted to an **excited** (higher) state it is temporary!!! The electron will fall back down to the ground state releasing light! (when viewed through a spectroscope-line emission spectra-gives a fingerprint of the atom)





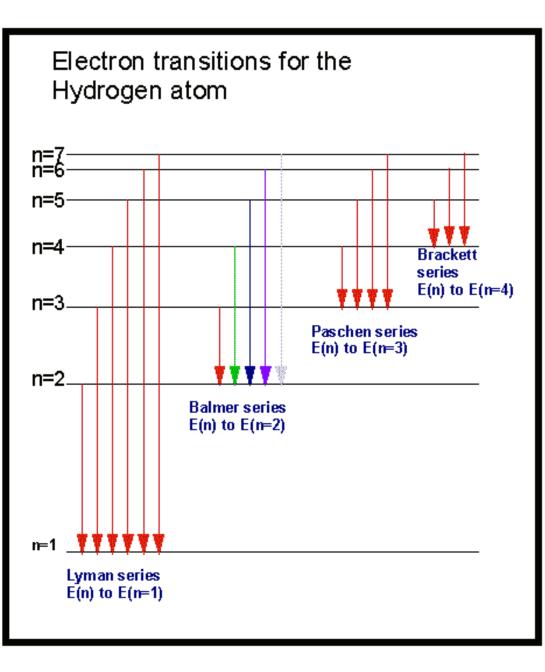
Spectroscopic analysis of the hydrogen spectrum...

produces a "bright line" spectrum

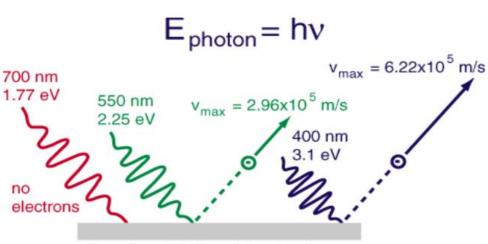


Electron transitions involve jumps of definite amounts of energy.

This produces bands of light with definite wavelengths.

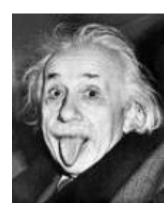


How does light behave as a particle?



Potassium - 2.0 eV needed to eject electron

Photoelectric effect



 Photoelectric effectwhen light of a particular frequency hits the surface of a metal an electron is ejected off the surface!

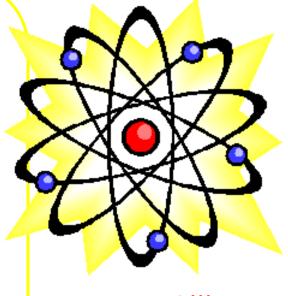
The Bohr Model of the Atom



Neils Bohr

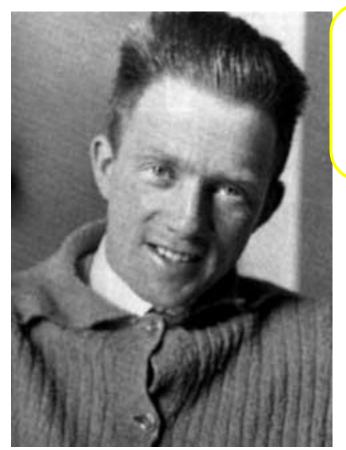
I pictured electrons orbiting the nucleus much like planets orbiting the sun.

But I was wrong! They're more like bees around a hive



WRONG!!!

Heisenberg Uncertainty Principle



Werner Heisenberg "One cannot simultaneously determine both the position and momentum of an electron."

You can find out where the electron is, but not where it is going.

You can find out where the electron is going, but not where it is!

Electron Configuration

Simplest way to write which energy levels and sublevels are filled within the atom (How many e⁻ and where you can find them)

How do electrons fill in an atom? The Diagonal Rule



• Sublevel # of electrons held

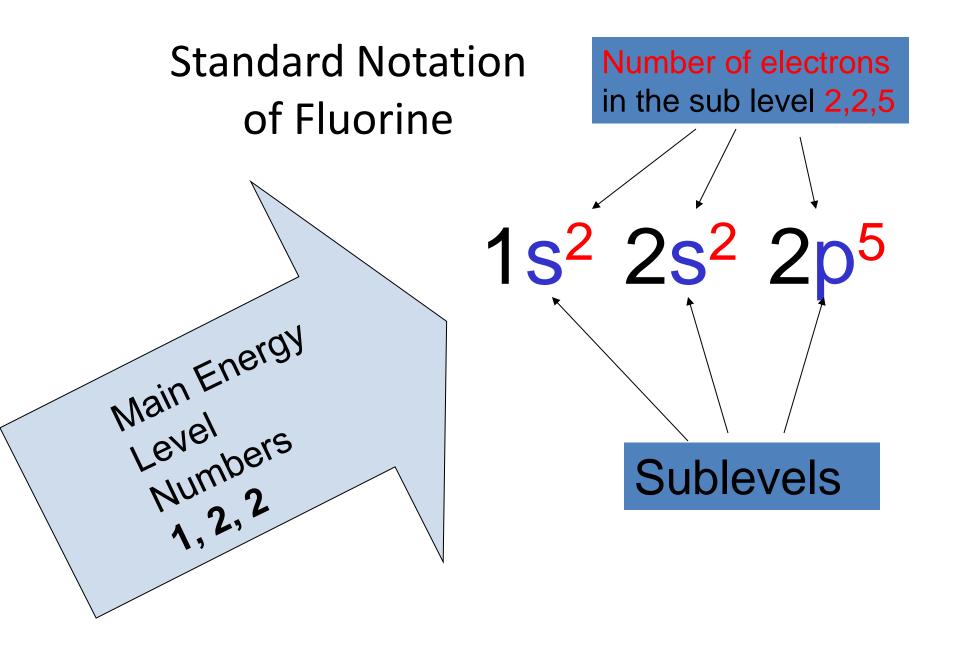
S 2 P 6

•

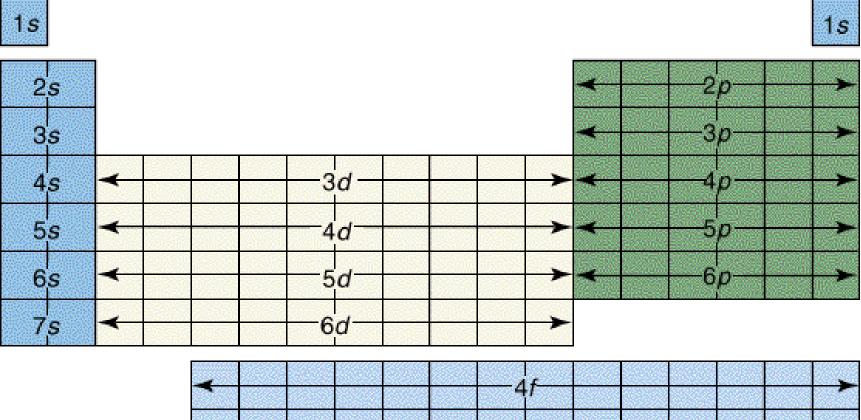
- D 10
- F 14

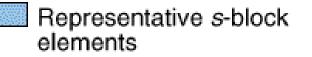
How to fill

- 1 Find total # of electrons
- 2 Write subshells in order of diagonal rule
- 3. Fill in subshells till all electrons are used
- 4. Last subshell may be partially filled.



Blocks in the Periodic Table





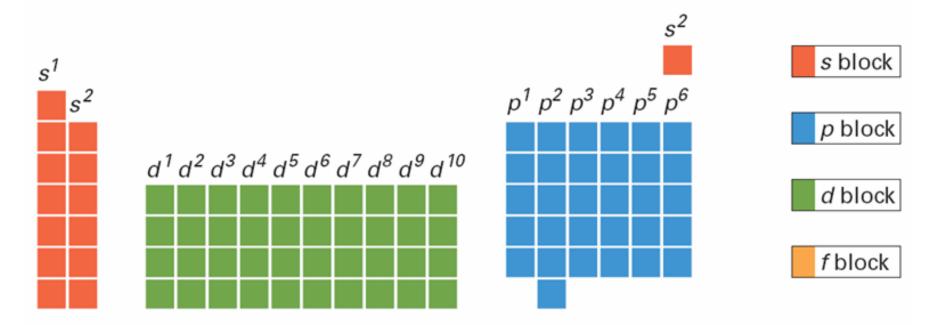
Transition metals





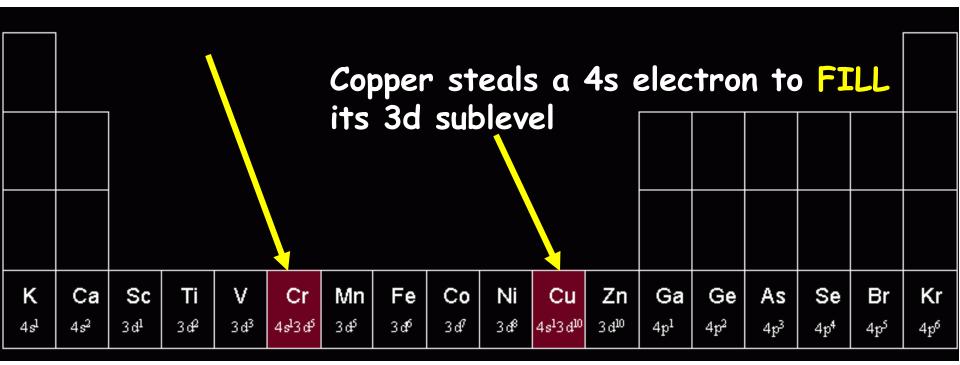
f-Block metals

5f



<u>Irregular conformations of Cr and Cu</u> <u>THE DEVIANT Ds</u>

Chromium steals a 4s electron to half fill its 3d sublevel (more stable)



	ŝ	Alkalin	e .													33 3		Noble gașes
	1 earth metals								Period			Halogens 1 ₈						
ĺ	1 H	1 2 2A	G	Group or Family								13 3A	14 4A	15 5A	16 6A	17 7A	2 He	
	3 Li	4 Be	Ļ											6 C	7 N	8 O	9 F	10 Ne
	11 Na	12 Mg	3	3 4 5 6 7 8 9 Transition metals							11	12	13 Al	14 (5)	15 P	16 S	17 Cl	18 Ar
Alkali metals	19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
	37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 	54 Xe
	55 Cs	56 Ba	57 La*	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 TI	82 Pb	83 Bi	84 Po	85 At	86 Rn
	87 Fr	88 Ra	89 Ac†	104 Unq	105 Unp	106 Unh	107 Uns	108 Uno	109 Une	110 Uun	111 Uuu							
*Lanthanides 58 59 60 61 Ce Pr Nd Pm					62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu				

97 Bk

98 Cf

99 Es

100

Fm

101

Md

102

No

103

Lr

† Actinides

90 Th

91 Pa

92 U

93

Np

94

Pu

95

Am

96

Cm

Alkali metals

Noble Gas Electron Configuration

- Even shorter way to write how electrons are distributed in atom
- Neon 1s²2s²2p⁶
- Aluminum 1s²2s²2p⁶3s²3p³

- Shows all electrons in shells common to a Noble Gas as the symbol in a bracket [symbol] then list leftover electrons in their energy levels and shells
- As you can see Al has the same distribution of inner electrons as neon therefore it can be written as:
- [Ne]3s²3p³

Steps for Noble Gas Configuration

- 1 Find element on periodic table.
- 2 Find number of electrons
- 3 Find Group 8 element from period above target element
- 4 Write group 8 element symbol in [brackets]
- **5 Subtract noble gases electrons from initial elements**
- 6 Start filling from S subshell of initial elements period # til all electrons are placed

<u>Element</u>	Configuration notation	Orbital notation	<u>Noble gas</u> <u>notation</u>
Lithium	1s²2s¹	1 2 2 2 2 2 2 2 2 2 2	[He]2s ¹
Beryllium	1s²2s²	$\frac{1}{1s}$ $\frac{1}{2s}$ $\frac{1}{2p}$ $\frac{1}{2p}$	[He]2s ²
Boron	1s²2s²p¹	$\begin{array}{c c} \uparrow & \uparrow & \uparrow \\ \hline 1s & 2s & \hline 2p & \\ \end{array}$	[He]2s²p¹
Carbon	1s²2s²p²	$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	[He]2s²p²
Nitrogen	1s²2s²p³	$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	[He]2s²p³
Oxygen	1s²2s²p⁴	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	[He]2s²p⁴
Fluorine	1s²2s²p⁵	$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	[He]2s²p⁵
Neon	1s²2s²p ⁶	$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	[He]2s²p ⁶

Orbital Notation or Diagrams

Simply use horizontal or vertical lines and arrows instead of exponents to represent the electrons

1 arrow = 1 electron Each line holds 2 electrons

of lines for S P D F must hold same number of electrons as in longhand electron configuration

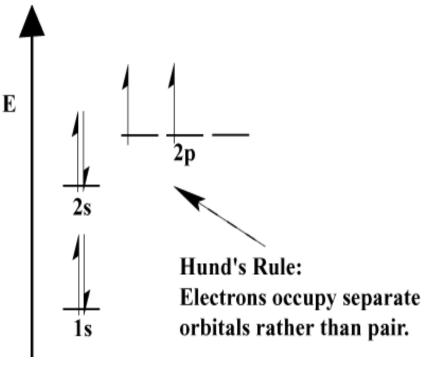
 $S = 2e^{-}$ so 1 line $P = 6e^{-}$ so 3 lines $d=10e^{-}$ so 5 lines

 $f = 14e^{-}$ so 7 lines

$$\frac{\uparrow\downarrow}{1s} \stackrel{\uparrow\downarrow}{=} \frac{\uparrow\downarrow}{2s} \stackrel{\uparrow\downarrow}{=} \frac{\uparrow\downarrow}{2p} \stackrel{\uparrow\downarrow}{=} \frac{\uparrow\downarrow}{3s} \stackrel{\uparrow}{=} \frac{\uparrow}{3p} = =$$

Rules for electron filling:

- Aufbaus Rule- must fill the lowest energy level available first!
- Hunds Rule -orbitals of equal energy sublevel will be occupied by one electron before a second one may enter (pairing up)
 - No one can have seconds until everyone from same row has gone through once!!



Pauli Exclusion Principle



Wolfgang Pauli Two electrons occupying the same orbital must have opposite spinsthis eliminates 2 electrons within the same atom having the same QNS

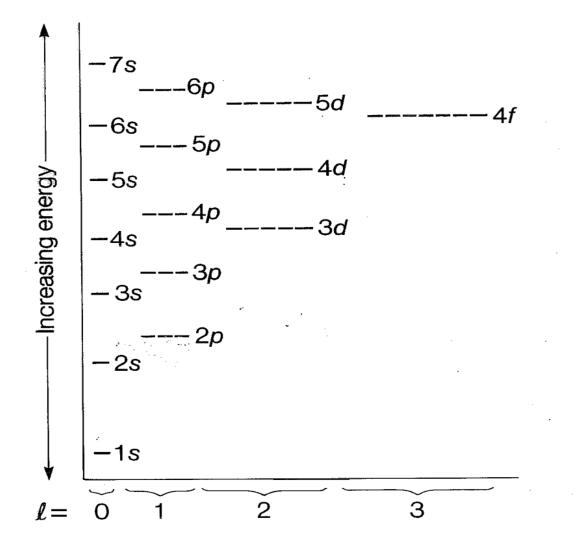
How do electrons fill in an atom? The Diagonal Rule



Things you must accept to do orbital Diagrams (energy diagrams)

- Energy builds further away from the nucleus
- Each line represents an orbital
- Each orbital can hold only two electrons
- We as a group will decide to place positive spin arrows in first..this is arbitrary NOT A RULE Just so all our QNS are the same
- Each electron is represented by an arrow
- In an orbital the two electrons must point in different directions
- Remember from the diagonal rule 4s fills before 3d breaking Aufbau's Rule

Orbital Diagrams



Energy Levels, Sublevels, Electrons

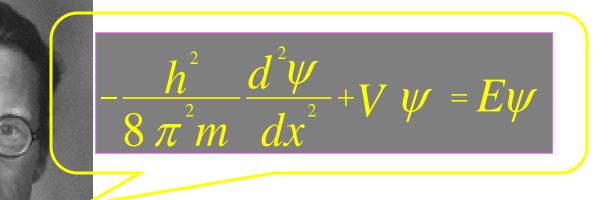
Energy Level (<i>n</i>)	Sublevels in main energy level (<i>n</i> sublevels)	Number of orbitals per sublevel	Number of Electrons per sublevel	Number of electrons per main energy level (2 <i>n</i> ²)
1	S	1	2	2
2	s p	1 3	2 6	8
3	s p d	1 3 5	2 6 10	18
4	s p d f	1 3 5 7	2 6 10 14	32

Quantum Mechanical Model of the Atom

Mathematical laws can identify the regions outside of the nucleus where electrons are most likely to be found.

These laws are beyond the scope of this class...VERY SIMPLY PUT... each electron has four numbers to describe the probability of finding the electron within the atom...

Schrodinger Wave Equation



Equation for <u>probability</u> of a single electron being found along a single axis (x-axis)

Erwin Schrodinger

What are they?

- Characterization of the orbital that an electron occupies
- Describes the following:
 - distance from the nucleus
 - shape
 - position with respect to the 3 dimensional axis
 - direction of spin of the electron

4 Quantum Numbers

n= Principle Quantum Number distance from the nucleus (Denotes Size) values 1-7 (note 7 periods on the P.T.) L = Sublevelshape of the cloud values $0 \rightarrow 3$ (0 = s, 1 = p, 2 = d, 3 = f) m = magnetic orientation about the axis values $-3 \rightarrow 3$ S= spin

Direction of movement within orbital

+ $\frac{1}{2}$ or $-\frac{1}{2}$

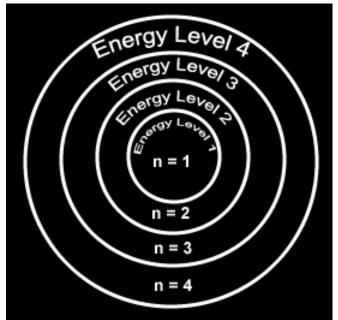
Electron Energy Level (Shell)

Generally symbolized by n, it denotes the probable distance of the electron from the nucleus.

n is numerically represented by positive integers. (1-7)

Number of electrons that can fit in a shell:

2n²

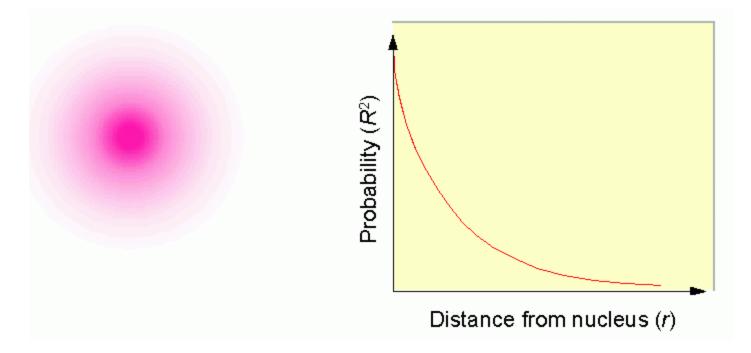


Angular Momentum

- · Abbreviated by ℓ
- Describes the shape of an orbital by using a number and letter designation.
- Determined by all values between
- (n-1) through 0

l	Letter
0	S
1	р
2	d
3	f

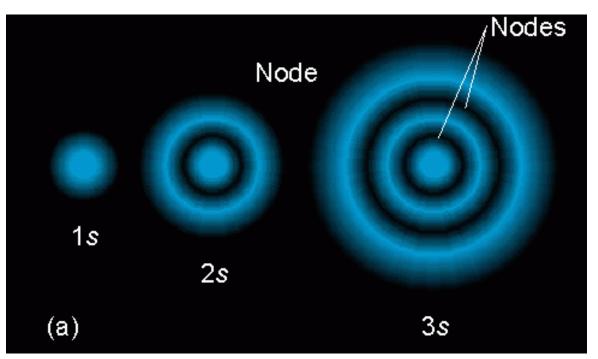
There are predicted shapes out to ℓ =6 Which would be a i orbital but don't exsist in nature. An orbital is a region within an energy level where there is a probability of finding an electron. This is a probability diagram for the s orbital in the <u>first</u> <u>energy level...</u>



<u>Orbital shapes</u> are defined as the surface that contains <u>90%</u> of the total electron probability.

<u>Sizes of s orbitals</u>

Orbitals of the same shape (s, for instance) grow larger as n increases...

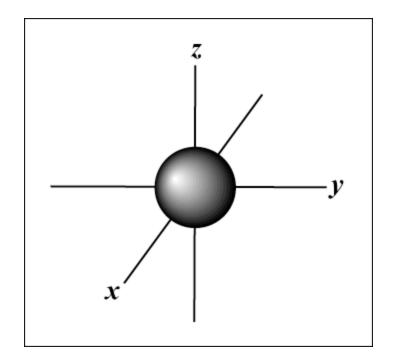


Nodes are regions of low probability within an orbital.

Shapes

- s orbital is spherical
- p orbital looks like a dumbell
- d orbitals look like 2 dumbells
- $\boldsymbol{\cdot}$ f orbitals look like flowers

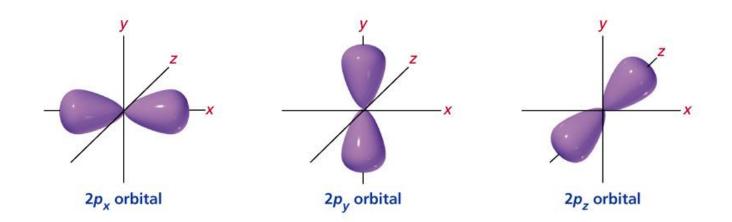
The s orbital has a spherical shape centered around the origin of the three axes in space.

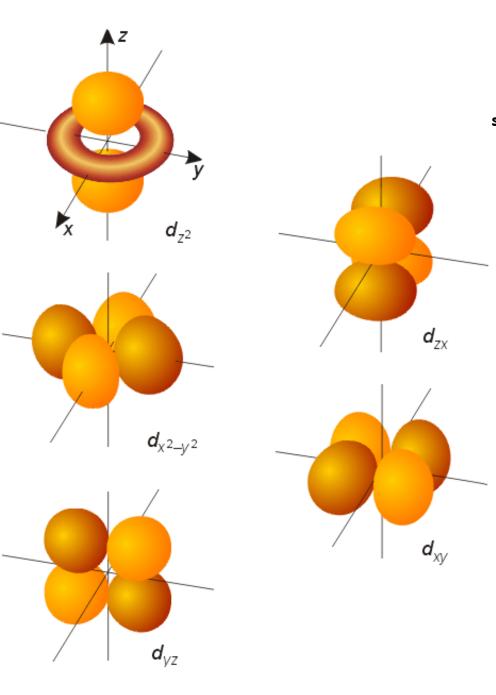


s orbital shape

P orbital shape

There are three dumbbell-shaped p orbitals in each energy level above n = 1, each assigned to its own axis (x, y and z) in space.

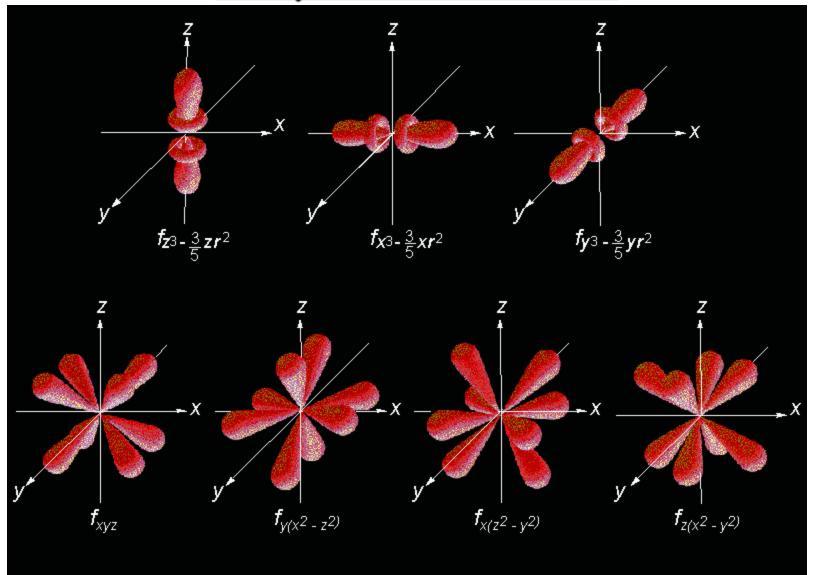




Things get a bit more complicated with the five d orbitals that are found in the d sublevels beginning with n = 3. To remember the shapes, think of "double dumbells"

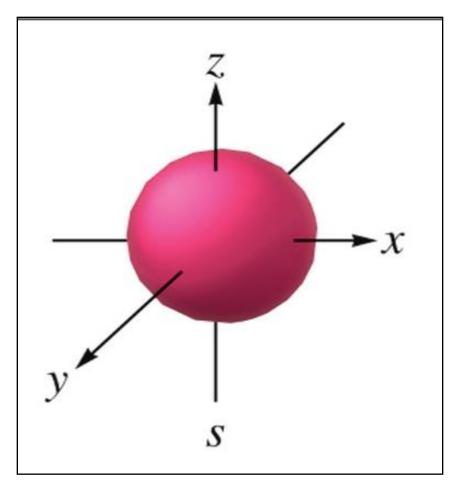
> ...and a "<u>d</u>umbell with a <u>d</u>onut"!

<u>Shape of f orbitals</u>

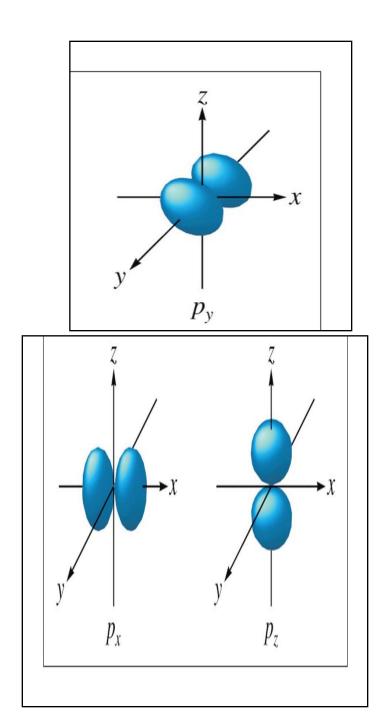


Magnetic Quantum Number

- · Abbreviated by m_l or simply m
- Represents the 3 dimensional orientation of an orbital (how your orbital is pointed)
- Assumes all values from $-\ell ... 0 ... + \ell$



- If n=1
- Then $\ell=0$
- So m_l=0
 - Think of spinning a basketball on your finger...does it really change where it is in 3D??



- For a p orbital...
 - n=2
 - *l*=1

$$-m_{l}=-1, 0, +1$$

 The p orbital can exist in different planes in 3D

Spin Quantum Number

- Abbreviated by m_s or s
- Uses +1/2 or -1/2
- $\boldsymbol{\cdot}$ Indicates the direction of spin of an electron
- Electrons in the same orbital MUST have opposite spins!

