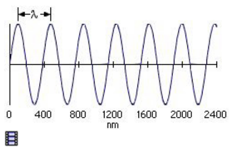
1

Electromagnetic Radiation

- Most subatomic particles behave as PARTICLES and obey the physics of waves.



Syllabus Learning Outcomes : 12

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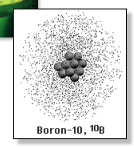
2

ATOMIC STRUCTURE

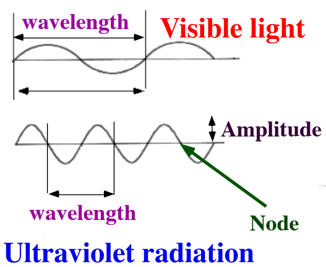


3

ELECTROMAGNETIC RADIATION

4

Electromagnetic Radiation



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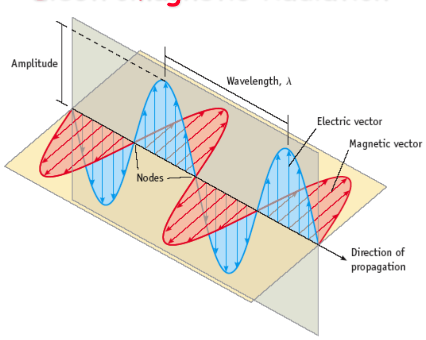
Electromagnetic Radiation



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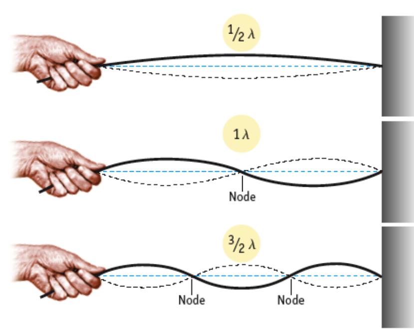

Wave motion: wave length and nodes

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Electromagnetic Radiation

- Waves have a frequency
- Use Greek letter "nu", ν, for frequency, and units are "cycles per sec" or hertz
- All radiation: $\lambda \cdot \nu = c$
- c = velocity of light = 3.00 x 10^8 m/sec
- Long wavelength --> low frequency
- Short wavelength --> high frequency

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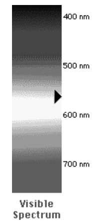
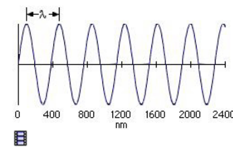
Electromagnetic Radiation

Long wavelength --> low frequency
Short wavelength --> high frequency





increasing frequency

increasing wavelength

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Electromagnetic Radiation

Red light has λ = 700 nm. Calculate the frequency.

$$700 \text{ nm} \cdot \frac{1 \times 10^{-9} \text{ m}}{1 \text{ nm}} = 7.00 \times 10^{-7} \text{ m}$$

$$\text{Freq} = \frac{3.00 \times 10^{8} \text{ m/s}}{7.00 \times 10^{-7} \text{m}} = 4.29 x 10^{14} \text{ s}^{-1}$$

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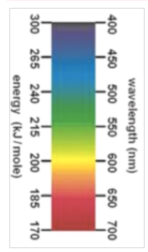
Electromagnetic Radiation



Short wavelength -->
high frequency
high energy

Long wavelength -->
low frequency
low energy

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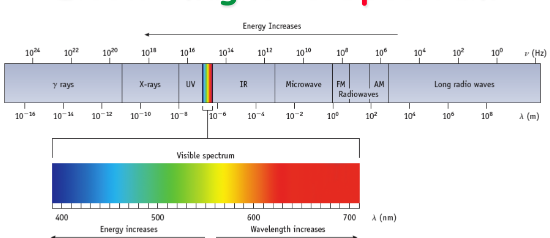
Electromagnetic Spectrum



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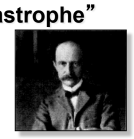
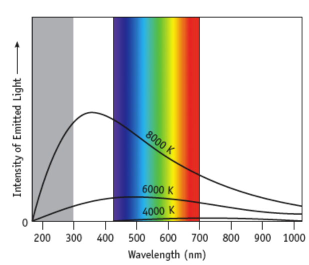
Quantization of Energy

Max Planck (1858-1947)
Solved the "ultraviolet catastrophe"



In the UV, intensity drops



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Quantization of Energy

An object can gain or lose energy by absorbing or emitting radiant energy in QUANTA.

Energy of radiation is proportional to frequency

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

h = Planck's constant = 6.6262×10^{-34} J•s

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Quantization of Energy

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

Light with long λ (low ν) has a low E.

Light with a short λ (high ν) has a high E.

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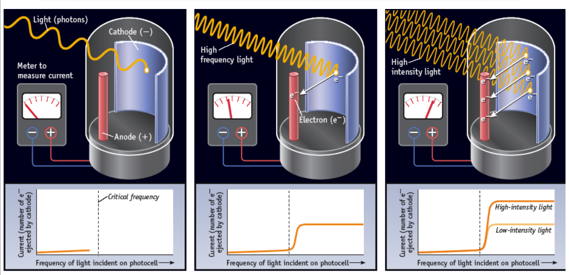
Photoelectric Effect

Experiment demonstrates the particle nature of light.



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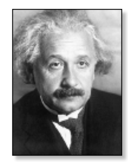
Photoelectric Effect

Classical theory said that E of ejected electron should increase with increase in light intensity—not observed!

- No e^- observed until light of a certain minimum E is used.
- Number of e^- ejected depends on light intensity.



A. Einstein (1879-1955)

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Photoelectric Effect

Understand experimental observations if light consists of particles called PHOTONS of discrete energy.

PROBLEM: Calculate the energy of 1.00 mol of photons of red light.

λ = 700. nm

ν = 4.29×10^{14} sec^{-1}

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Energy of Radiation

Energy of 1.00 mol of photons of red light.

E = h•ν

= $(6.63 \times 10^{-34}$ J•s$)(4.29 \times 10^{14}$ s$^{-1})$

= 2.85×10^{-19} J per photon

E per mol =

$(2.85 \times 10^{-19}$ J/ph$)(6.02 \times 10^{23}$ ph/mol$)$

= 171.6 kJ/mol

This is in the range of energies that can break bonds.

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Explain QT

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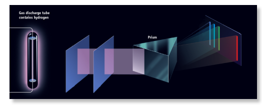
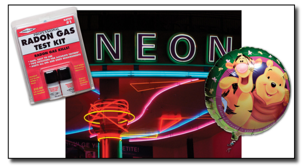
Excited Atoms & Atomic Structure





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Atomic Line Emission Spectra and Niels Bohr

Niels Bohr

(1885-1962)

Bohr's greatest contribution to science was in building a simple model of the atom. It was based on an understanding of the **SHARP LINE EMISSION SPECTRA** of excited atoms.

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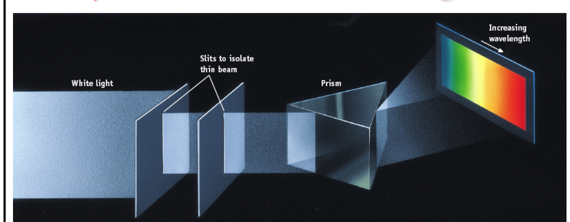
Spectrum of White Light



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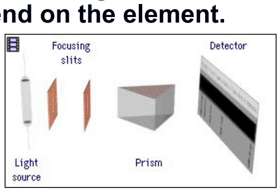
Line Emission Spectra of Excited Atoms

- Excited atoms emit light of only certain wavelengths
- The wavelengths of emitted light depend on the element.



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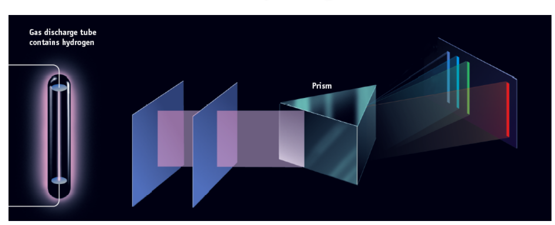
Spectrum of Excited Hydrogen Gas



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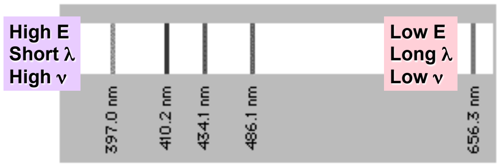
Line Emission Spectra of Excited Atoms

Atomic Line Spectrum of Excited H Atoms



Visible lines in H atom spectrum are called the BALMER series.

For H, electron transitions n=? to n=2 are in visible λ

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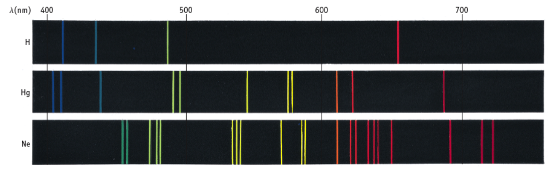
Line Spectra of Other Elements



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The Electric Pickle

- Excited atoms can emit light.
- Here the solution in a pickle is excited electrically. The Na^+ ions in the pickle juice give off light characteristic of that element.

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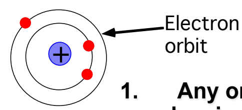
Atomic Spectra and Bohr

One view of atomic structure in early 20th century was that an electron (e-) traveled about the nucleus in an orbit.



1. Any orbit should be possible and so is any energy.
2. But a charged particle moving in an electric field should emit energy.

End result should be destruction!

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Atomic Spectra and Bohr

Bohr said classical view is wrong.

Need a new theory — now called QUANTUM or WAVE MECHANICS.

e- can only exist in certain discrete orbits — called stationary states.

e- is restricted to QUANTIZED energy states.

Energy of state = - C/n^2

where n = quantum no. = 1, 2, 3, 4, ...

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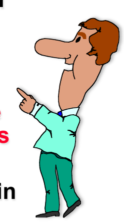
Atomic Spectra and Bohr

Energy of quantized state = - B/n^2



- Only orbits where n = integral no. are permitted.
- Radius of allowed orbitals = $n^2 \cdot (0.0529$ nm)
- But note — same eqns. come from modern wave mechanics approach.
- Results can be used to explain atomic spectra of hydrogen.

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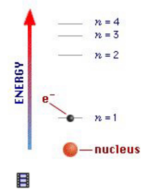
Atomic Spectra and Bohr

If e-'s are in quantized energy states, then ΔE of states can have only certain values. This explain sharp line spectra.

$$E = -\frac{C}{2^2} \quad n = 2$$

$$E = -\frac{C}{1^2} \quad n = 1$$



C = Rhc = 1312kj/mol

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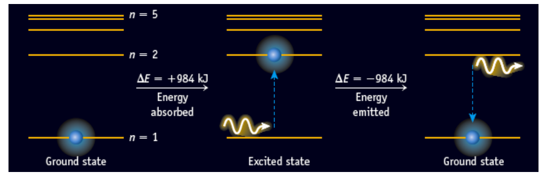
Energy Absorption/Emission



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Atomic Spectra and Bohr

ENERGY

$E = -C\,(1/2^2)$ n = 2

$E = -C\,(1/1^2)$ n = 1

Calculate ΔE for e- "falling" from high energy level (n = 2) to low energy level (n = 1).

$\Delta E = E_{final} - E_{initial} = -C[(1/1^2) - (1/2^2)]$

ΔE = -(3/4)C

Note that the process is **EXOTHERMIC**

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Atomic Spectra and Bohr

ENERGY

$E = -C\,(1/2^2)$ n = 2

$E = -C\,(1/1^2)$ n = 1

ΔE = -(3/4)C E = hv

C has found from experiment (and is now called **R**, the **Rydberg** constant)

R (= C) = 1312 kJ/mol or 3.29×10^{15} cycles/sec

so, E of emitted light

= (3/4)R = 2.47×10^{15} sec^{-1}

and λ = c/ν = **121.6 nm**

This is exactly in agreement with experiment!

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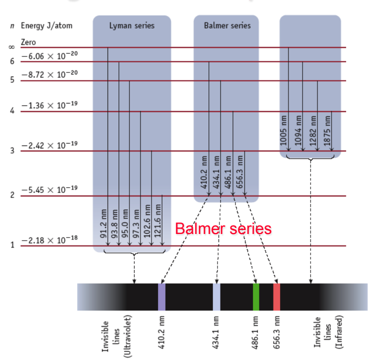
Origin of Line Spectra



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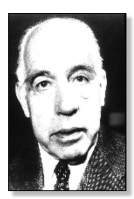
Atomic Line Spectra and Niels Bohr



Niels Bohr

(1885-1962)

Bohr's theory was a great accomplishment.

Rec'd Nobel Prize, 1922

Problems with theory —

- theory only successful for H.
- introduced quantum idea artificially.
- So, we go on to **QUANTUM** or **WAVE MECHANICS**

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Quantum or Wave Mechanics

L. de Broglie
(1892-1987)

de Broglie (1924) proposed that all moving objects have wave properties.

For light: $E = mc^2$

$E = h\nu = hc / \lambda$

Therefore, $\lambda = h / mc$

and for particles, $\lambda = h / mv$

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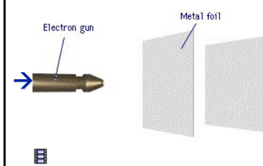
Quantum or Wave Mechanics



Experimental proof of wave properties of electrons

115g baseball (0.115kg) at 100 mph

$\lambda = 1.3 \times 10^{-32}$ cm

e- with velocity = 1.9×10^8 cm/sec

$\lambda = 0.388$ nm

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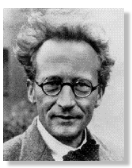
Quantum or Wave Mechanics



E. Schrodinger
1887-1961

Schrodinger applied idea of e- behaving as a wave to the problem of electrons in atoms.

He developed the WAVE EQUATION

Solution gives set of math expressions called WAVE FUNCTIONS, Ψ

Each describes an allowed energy state of an e-

Quantization introduced naturally.

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WAVE FUNCTIONS, Ψ

- Ψ is a function of distance and two angles (n, ℓ, m_ℓ).
- Each Ψ corresponds to an ORBITAL *— the region of space within which an electron is found.*
- Ψ does NOT describe the exact location of the electron.
- Ψ^2 is proportional to the probability of finding an e^- at a given point.

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Uncertainty Principle

W. Heisenberg
1901-1976

Problem of defining nature of electrons in atoms solved by W. Heisenberg.

Cannot simultaneously define the position and momentum (= m•v) of an electron.

We define e^- energy exactly but accept limitation that we do not know exact position.

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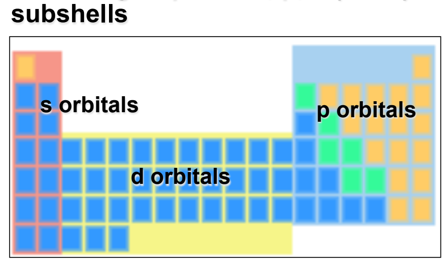
Orbitals

- No more than 2 e- assigned to an orbital
- Orbitals grouped in s, p, d (and f) subshells



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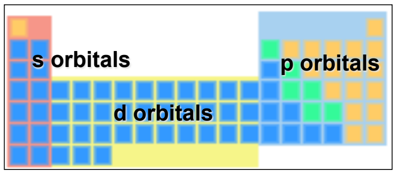

	s orbitals	p orbitals	d orbitals
# orbitals	1	3	5
# e-	2	6	10

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Subshells & Shells

- Subshells grouped in shells.
- Each shell has a number called the PRINCIPAL QUANTUM NUMBER, n
- The principal quantum number of the shell is the number of the period or row of the periodic table where that shell begins.

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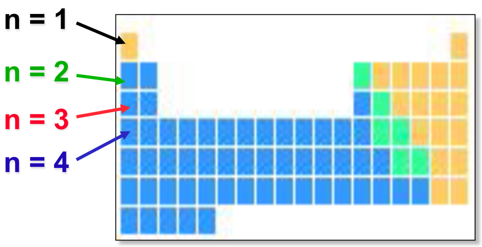
Subshells & Shells



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QUANTUM NUMBERS

The shape, size, and energy of each orbital is a function of 3 quantum numbers:

n (major) ---> shell (1,2,3,4,5,6,7,...)

ℓ (angular) momentum ---> subshell (shape)

m_ℓ (magnetic) ---> designates an orbital within a subshell (orientation)

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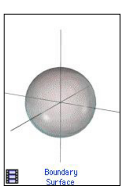
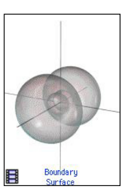
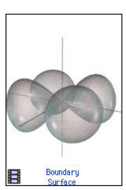
ℓ gives shape of orbital



s orbital
ℓ=0



p orbital
ℓ=1



d orbital
ℓ=2

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QUANTUM NUMBERS

Symbol	Allowed values	Description
n (major)	1, 2, 3, ..	Orbital size and energy where $E = -B/n^2$)
ℓ (angular)	0, 1, 2, .. n-1	Orbital shape or type (subshell)
m_ℓ (magnetic)	$-\ell..0..+\ell$	Orbital orientation

# of orbitals in subshell = $2\ell + 1$

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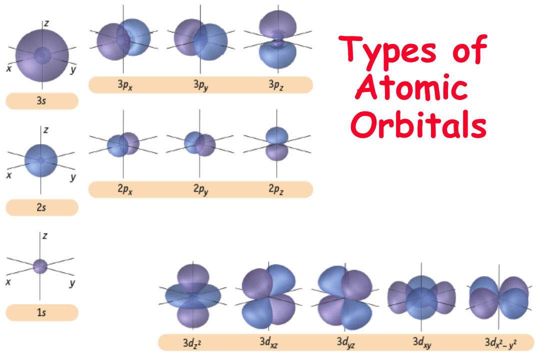

Types of Atomic Orbitals

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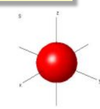
Shells and Subshells



When n = 1, then ℓ = 0 and m_ℓ = 0

Therefore, in n = 1, there is 1 type of subshell

and that subshell has a single orbital

(m_ℓ has a single value ---> 1 orbital)

This subshell is labeled **S** ("ess")

Each shell has 1 orbital labeled s, and it is *SPHERICAL* in shape.

H He

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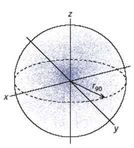
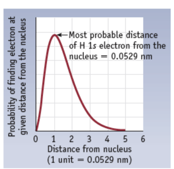
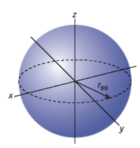
s Orbitals— Always Spherical







Dot picture of electron cloud in 1s orbital.

Surface density $4\pi r^2 \psi$ versus distance

Surface of 90% probability sphere

l=0 is an s orbital

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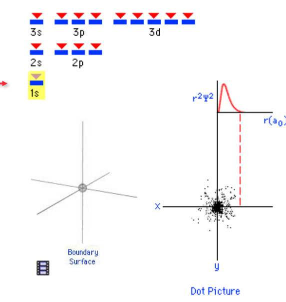
1s Orbital

H

He



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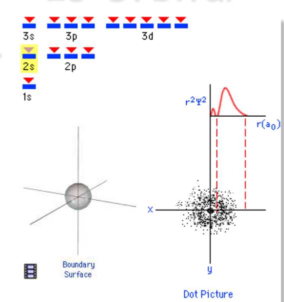
2s Orbital

Li

Be



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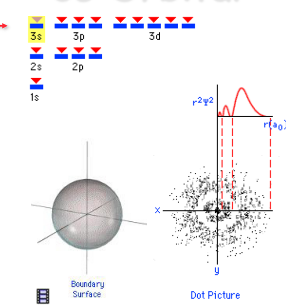
3s Orbital

Na

Mg



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p Orbitals

When n = 2, then ℓ = 0 and 1

Therefore, in n = 2 shell there are 2 types of orbitals — 2 subshells

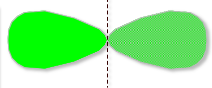
For $\ell = 0$ $m_\ell = 0$

this is an s subshell (2s)

For $\ell = 1$ $m_\ell = -1, 0, +1$

this is a **p subshell (2p)** with **3 orbitals**

Typical p orbital



When l = 1, there is a PLANAR NODE thru the nucleus.

Ne

Li Be B C N O F

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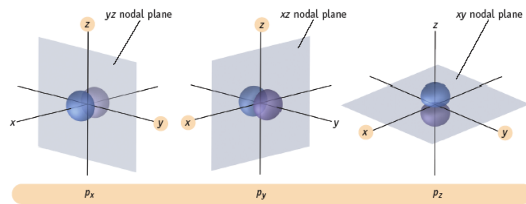
p Orbitals



The three p orbitals lie 90° apart in space

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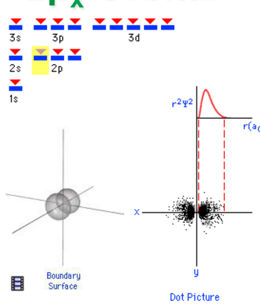
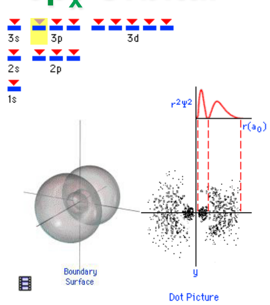
$2p_x$ Orbital



$3p_x$ Orbital



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d Orbitals

When n = 3, what are the values of ℓ?

ℓ = 0, 1, 2

and so there are 3 subshells in the shell.

For $\ell = 0$, $m_\ell = 0$

---> s subshell with single orbital

For $\ell = 1$, $m_\ell = -1, 0, +1$

---> p subshell with 3 orbitals

For $\ell = 2$, $m_\ell = -2, -1, 0, +1, +2$

---> **d subshell with 5 orbitals**

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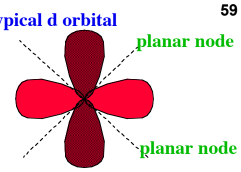
d Orbitals

typical d orbital

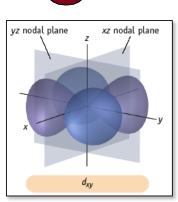


s orbitals have no planar node (l = 0) and so are spherical.

p orbitals have l = 1, and have 1 planar node,

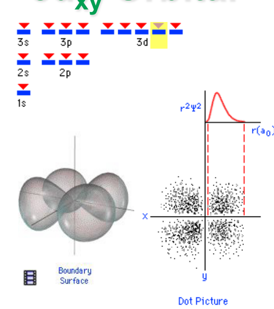
and so are “dumbbell” shaped.

This means d orbitals (with l = 2) have 2 planar nodes



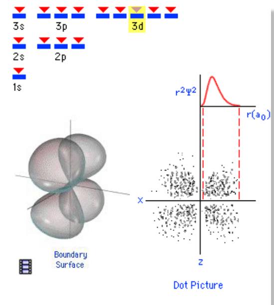
60

$3d_{xy}$ Orbital



61

$3d_{xz}$ Orbital



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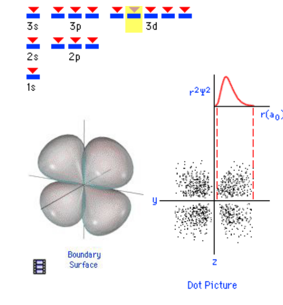
$3d_{yz}$ Orbital



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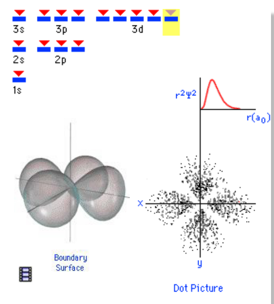
$3d_{x^2-y^2}$ Orbital



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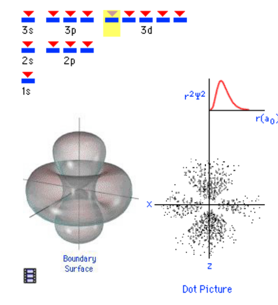
$3d_{z^2}$ Orbital



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f Orbitals

When n = 4, ℓ = 0, 1, 2, 3 so there are 4 subshells in the shell.

For $\ell = 0$, $m_\ell = 0$
---> s subshell with single orbital

For $\ell = 1$, $m_\ell = -1, 0, +1$
---> p subshell with 3 orbitals

For $\ell = 2$, $m_\ell = -2, -1, 0, +1, +2$
---> d subshell with 5 orbitals

For $\ell = 3$, $m_\ell = -3, -2, -1, 0, +1, +2, +3$
---> f subshell with 7 orbitals

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f — Orbitals

One of 7 possible f orbitals.

All have 3 planar surfaces.

Can you find the 3 surfaces here?

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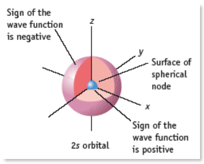
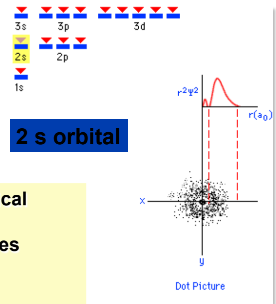
Spherical Nodes





- Orbitals also have spherical nodes
- Number of spherical nodes
  = n - l - 1
- For a 2s orbital:
  No. of nodes = 2 - 0 - 1 = 1