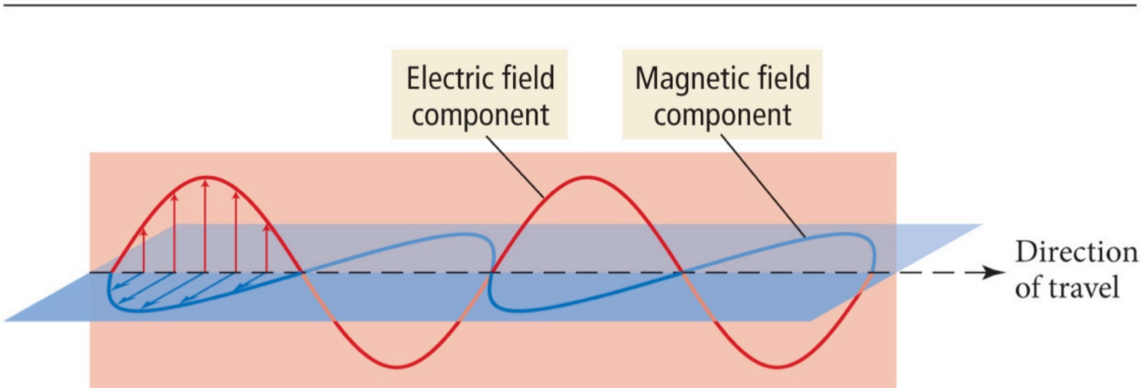
Reading Assignment Sections 7.1-7.6

The **quantum-mechanical model**

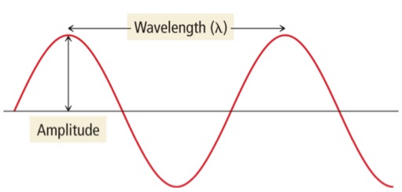
The Nature of Light: Its Wave Nature

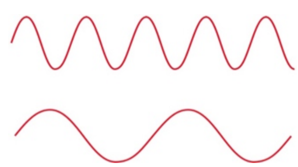
- Light: a form of **electromagnetic radiation**
  - Composed of perpendicular oscillating waves, one for the electric field and one for the magnetic field

Electromagnetic Radiation



Waves in nature:





The larger the amplitude, the brighter the light.

Frequency (*v frequency number of complete wavelengths or cycles which pass a given point per second)*

ν =

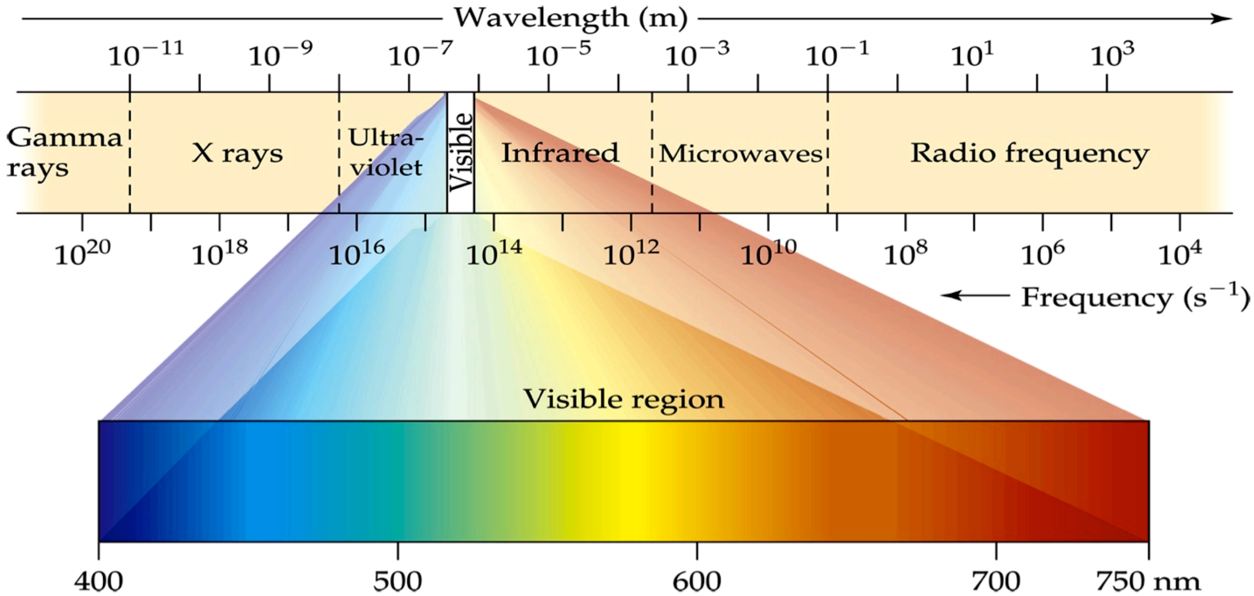
For waves traveling at the same speed, the shorter the wavelength, the more frequently they pass.

$$\nu = \frac{c}{\lambda}$$

C = Speed of light is constant = 3.00 X10^8 m/s.

λ = wave length (m)

The Electromagnetic Spectrum



- An argon ion laser emits light at 457.9 nm. What is the frequency of this radiation?

$6.547 \times 10^{14}\ s^{-1}$

- If an FM radio station broadcasts at 92.1 MHz, What is the wavelength of this radiation?

3.26 m

- *A plutonium-239 atom may emit a photon of light with a wavelength of 24.0 pm when it undergoes nuclear fission. What is the frequency of this radiation?*

$1.25 \times 10^{19}\ s^{-1}$

The *photoelectric effect* is the emission of electrons from metal surfaces on which light shines

Einstein used the idea of quanta to explain the photoelectric effect.
He assumed that light traveled in energy packets called **photons**.

- **energy is quantized**: It occurs in small "packets" or **quanta** of energy
  - the basis of quantum theory

A "packet" or **quantum** of energy is known as a **photon**, a very, very, very tiny amount of radiation
Photon: is an elementary particle. It is a quantum of light. Photons are bundles of light energy that is emitted by electrons as they go from higher energy levels to lower levels
Quantum: is the minimum amount of any physical entity in an interaction. A quantum of energy is the amount of energy required to move an electron from one energy level to another

★ The energy of **one photon** is $\boldsymbol{E = h\nu =}$ ***J/Photon***
★ Threshold frequency: $\boldsymbol{h\nu = \phi}$

h : Planck's constant = 6.63 x 10^{-34} J·s
ϕ = Binding energy of the emitted electron

A photon's energy must exceed a minimum threshold frequency for electrons to ejected

- ✓ Below the threshold frequency no electrons are ejected.
- ✓ Above the threshold frequency, the excess energy appears as the kinetic energy of the ejected electrons.

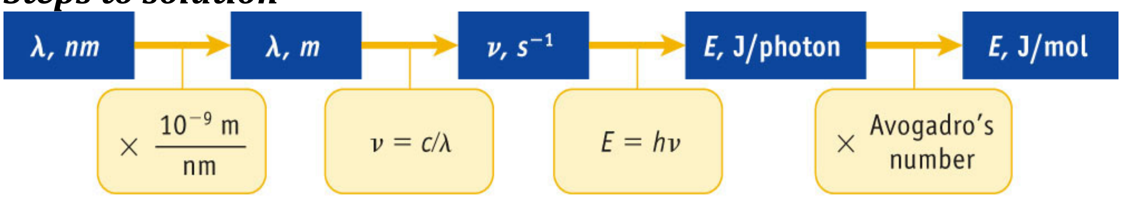
Kinetic Energy = $E_{photon} - E_{binding}$

$$KE = h\nu - \phi$$

***Remember 1 mol of anything has Avogadro's # of that thing
So 1mol light has __________ photons

In conclusion:
Light has a wavelike properties ⇒ continuous spectrum of colors for light
Light has particle like properties⇒ **photon** is a light particle.
E = hν ***and*** ***c = λ.ν***

So E =
Steps to solution



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- Calculate the energy of 1.00 mol of photons of red light.

$\lambda =$ 750. nm
ν = 4.29×10^{14} sec^{-1}

172 kJ/mol

- If the energy of 1.00 mole of photons is 346 kJ, what is the wavelength of the light?

346 nm

- Excited hydrogen atoms emit light in the infrared at 1.87×10^{-6} m. What is the energy of a single photon with this wavelength?

1.06×10^{-19} J

How about matter; does it have a wavelike properties?

- Louis de Broglie hypothesized that if light can have material properties, matter should exhibit wave properties.
- He demonstrated that the relationship between mass and wavelength was

deBroglie's Equation: $\lambda = h/mv$
m = mass in Kg
v = velocity (m/s)

- ✓ deBroglie's equation summarized the concepts of **waves and particles** as they apply to **low-mass**, **high-speed** objects.
- ✓ This is called wave-particle duality
- ✓ These are just models
- ✓ As a consequence of deBroglie's discovery, we now have techniques such as **X-ray diffraction** and **electron microscopy** to study small objects

- Calculate the de Broglie wavelength for a 907.2 kg car moving at a speed of 96.6 km/hr. h (6.63×10^{-34} J.s)

$\lambda = 2.72 \times 10^{-38}$ m

The Uncertainty Principle

Heisenberg's uncertainty principle: we cannot determine the *exact* position, direction of motion, and speed of subatomic particles simultaneously.

- **For electrons: we cannot determine their momentum (= m•v) and position simultaneously.:**

  $(\Delta x)(\Delta mv) \geq h/4\pi$

  - Calculate the uncertainty in the position of an electron moving at a speed of (3.30 ± 0.01) x 10^5 m/s (Take the mass of the electron m = 9.109 x 10^{-31} Kg.)

    6 x 10^{-8} m

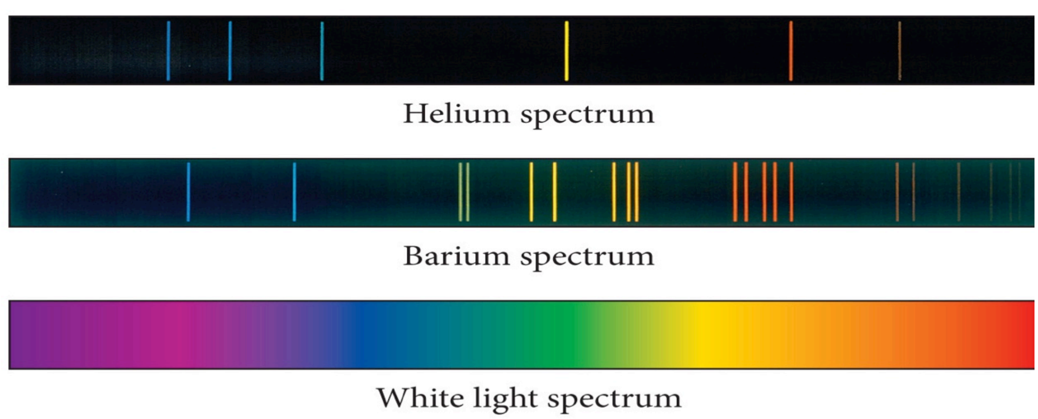
  - An electron (mass= 9.109X$10^{-31)}$ has an uncertainty in its position of 450pm . What is the uncertainty in its velocity?

    1.28X10^5 m/s

Atomic spectroscopy:

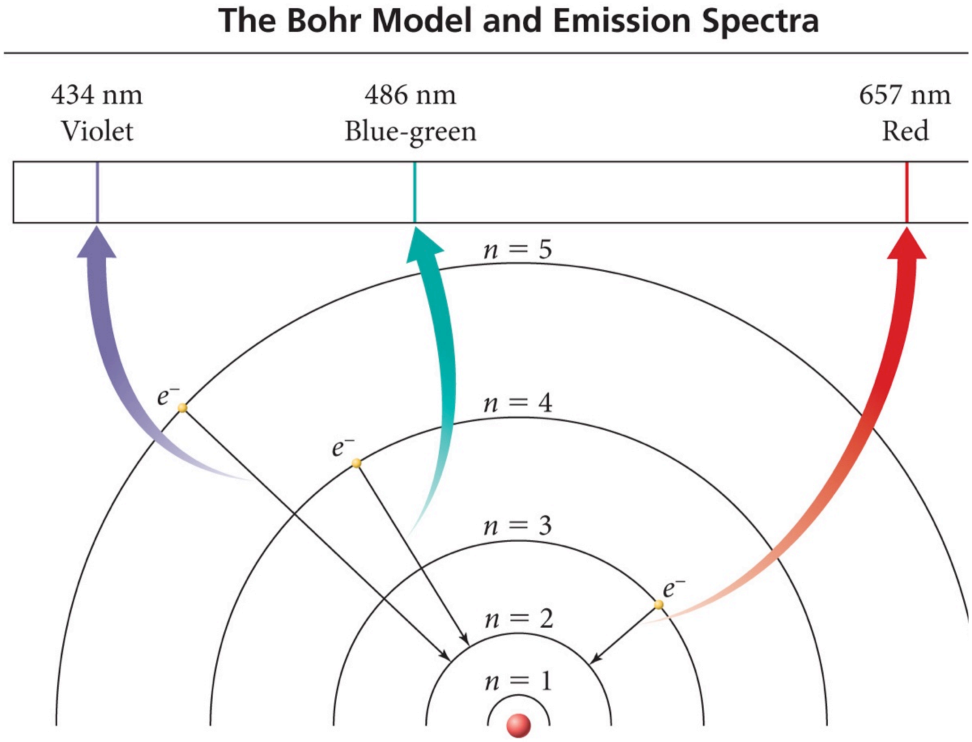
★ When atoms or molecules absorb energy, that energy is often released as light energy, Fireworks, neon lights, etc

Examples of Spectra



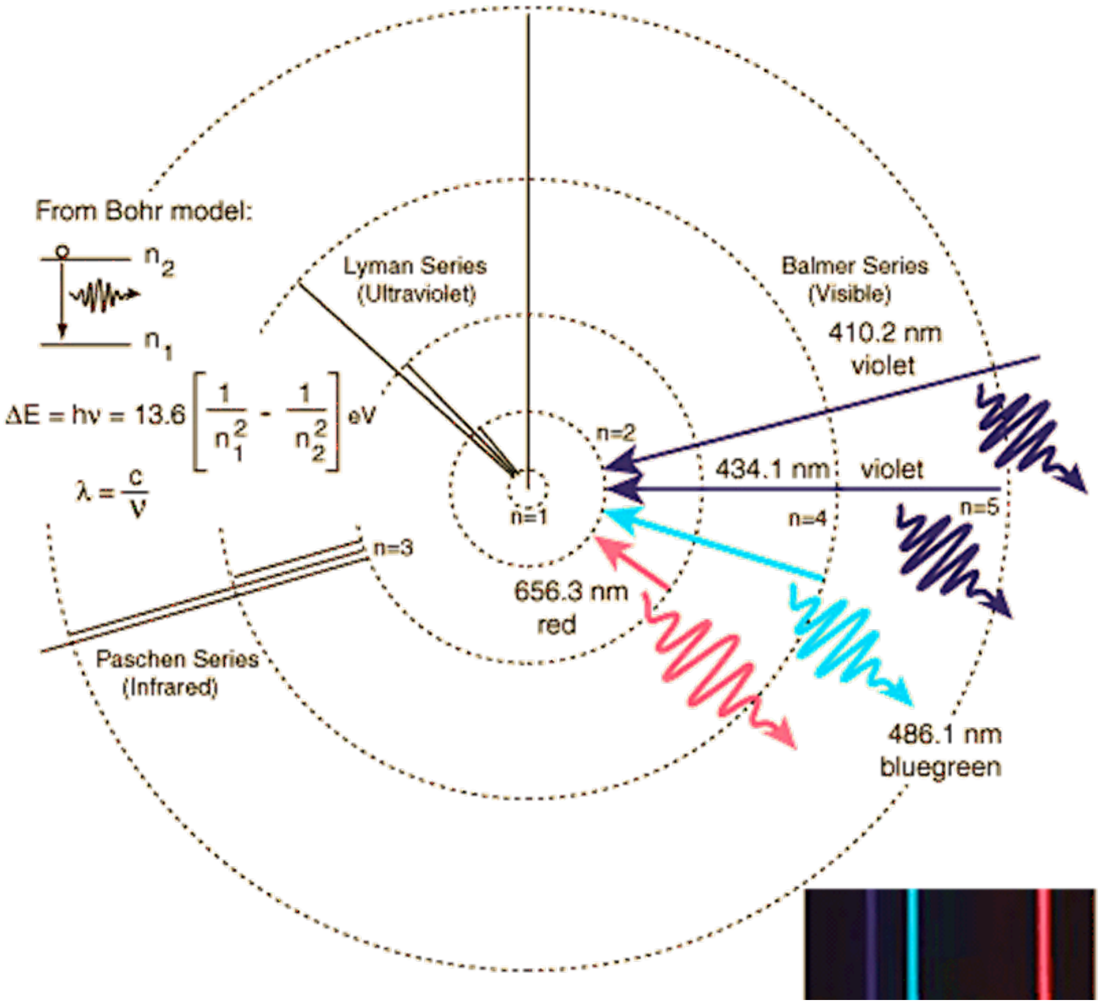
(b)

Bohr Model of H Atom



- ✓ Electrons orbit the nucleus
- ✓ Only specific orbits are possible
- ✓ Kinetic energy of attraction between positive protons and negative electrons.
  - **Energy Levels & Orbits:** Electron is restricted to certain energy levels corresponding to spherical orbits, with certain radii, about the nucleus

- Electrons will be at the lowest energy level available (ground state)
- When energy is provide, the electron absorbs the energy and jumps to higher energy levels, farther from nucleus (Excited State)
- The amount of light energy added must exactly match the energy change between the two levels
- Electron does not stay excited it falls back to the Ground state and thus - emits the energy diff. as light



Many transitions are possible each goes with a unique **ΔE**

$$\Delta E_{electron} = E_{final\ state} - E_{initial\ state}$$

$$\mathbf{E_{photon} = -\Delta E_{electron} = -\Delta E_{emission} = h\,\nu} = h\frac{c}{\lambda}$$

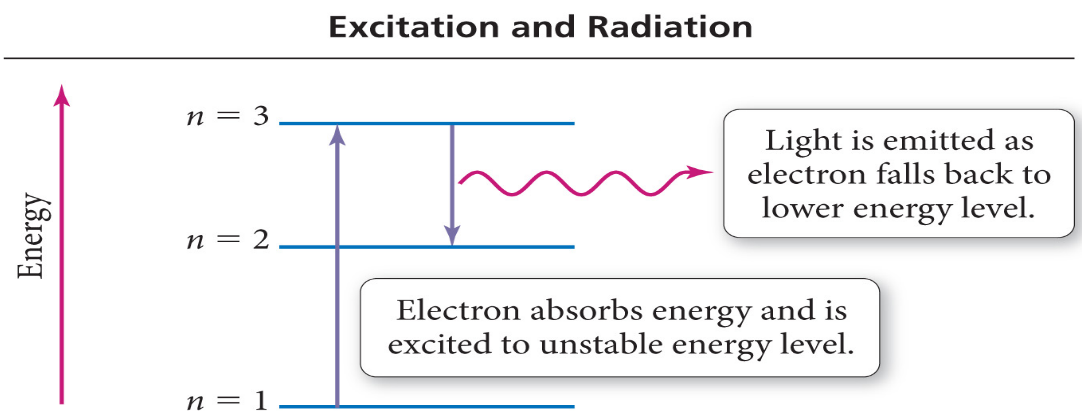
- Remember: **Photons** are bundles of light energy that is emitted by electrons as they go from higher energy levels to lower levels.

★ Note: most negative energy represents most stable state

Energy of a photon emitted
when e- "drops" to a lower energy level is related to frequency (wavelength) of radiation

$$\Delta E = -2.18 \times 10^{-18} \left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right)$$

✓ n_i and n_f are the initial and final energy levels of the electron.

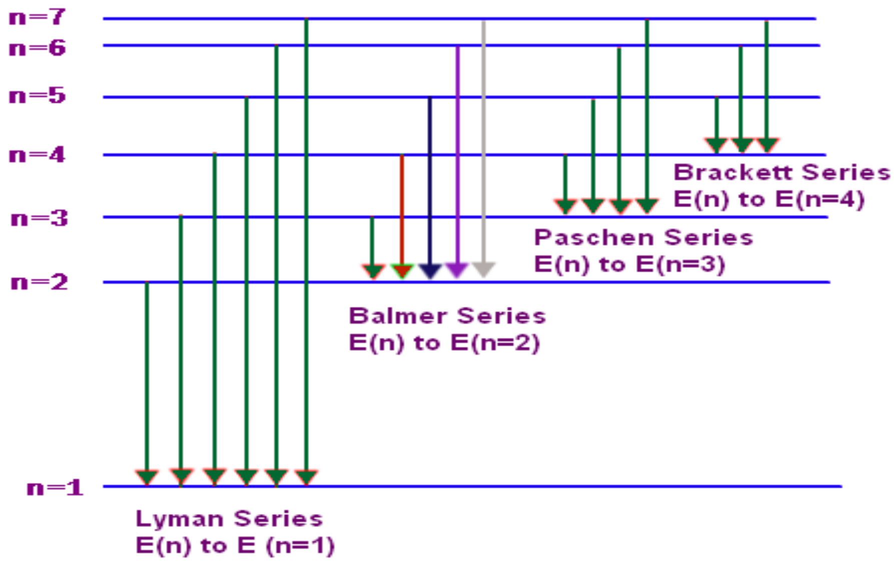


� For a hydrogen atom, calculate the energy of a photon in the line spectra that results from the transition
$n = 3$ to $n = 2$.

★ In a line spectrum, the wave lengths of light emitted can be calculated using Rydberg equation (will be used in lab)

$$\frac{1}{\lambda} = R\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right)$$

R = 1.0974 x 10 ^{7} m^{-1}



� Calculate. the wavelength (nm) and energy (KJ/mol) of the second line in the Balmer series. In what region of the electromagnetic spectrum does it fall?

$4.0875 \text{ X } 10^{-19}$ J

$4.87 \text{ X} 10^{-7}$ m

Studies still going!!!
Boher model, Balmer, Rydberg work well for the hydrogen atom but not for multi electrons atoms??????

- ✓ Remember uncertainty principle (Heisenberg)

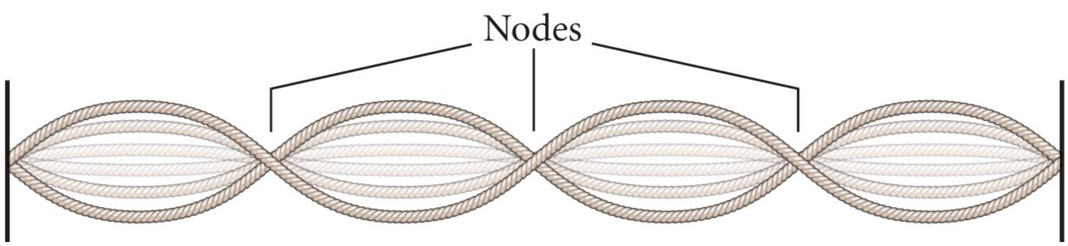
★ Schrodinger developed a compromise which calculate both energy of an electron and the probability of finding an electron at any point I the molecule or atom

- ➢ Erwin Schrödinger proposed an equation containing both **wave** and **particle** terms
- ➢ The wave function ***psi*** **(ψ)** describes

the electron's matter wave

- ✓ Each ψ corresponds to a specific energy & describes a region about the nucleus, an orbital, in which an e- with that energy may be found
- ✓ ψ^2, gives the **probability of finding the electron.**
- ✓ ψ^2 is called the **probability density** or **Electron density**

Nodes in the functions are where the probability to find an electron is **ZERO**



Quantum Numbers: Solutions to the Schrodinger Eqn for Hydrogen atom

- Solving the wave equation gives a set of wave functions, or orbitals, and their corresponding energies and locations
- An orbital is described by a set of **four quantum numbers**

n **ℓ** **m_ℓ** **m_s**

1-Principal Quantum Number (*n*)

- The principal quantum number, *n*, describes the energy level on which the orbital resides and accordingly the size.
- The values of *n* are integers ≥ 1.
- The larger the value of *n*, the larger the orbital and the more energy the orbital has.
- As *n* gets larger, the amount of energy between orbitals gets smaller

2- Angular Momentum Quantum Number **(ℓ)** "Azimuthal"

- This quantum number defines the **shape** of the orbital.
- Allowed values of ℓ are integers ranging from
- **0 to n – 1**.

Value of ℓ				
Type of orbital				

n	Possible sub-shells (ℓ)	Possible sub-shells (ℓ)
n = 1 (1st shell)	ℓ =	ℓ =
n = 2 (2nd shell)	ℓ = 0 or 1	ℓ = s or p
n = 3 (3rd shell)	ℓ = 0 or 1 or 2	ℓ = s or p or d
n = 4 (4th shell)	ℓ = 0 or 1 or 2 or 3	ℓ = s or p or d or f

3- Magnetic Quantum Number **(m_l)**

- The magnetic quantum number describes the **three-dimensional orientation of the orbital**.
- Allowed values of m_l are integers ranging from

  - ℓ to + ℓ Including zero

Each number m_l represents one **orbital**

L (sub-shell)	sub-sublevel (ml)	# of orbitals	orbitals
l = 0	ml = 0	1	s
l = 1	ml = -1,0,1	3	p_x, p_y, p_z
l = 2	ml = -2,-1,0,1,2	5	d_{xy}, d_{yz}, d_{xz}, $d_{x^2-y^2}$, d_{z^2}
l = 2	ml = -3,-2,-1,0,1,2, 3	7	f (7 orbitals

4- Spin Quantum Number, m_s

The spin quantum number , ms has only 2 allowed values: +1/2 and −1/2.

- The experiment reveals that the electrons spin on their axis.
- As they spin, they generate a magnetic field.
  - Spinning charged particles generates a magnetic field.
- If there is an even number of electrons, about half the atoms will have a net magnetic field pointing "north" and the other half will have a net magnetic field pointing "south.

TABLE 6.1 Summary of the Quantum Numbers, Their Interrelationships, and the Orbital Information Conveyed

Principal Quantum Number	Azimuthal Quantum Number	Magnetic Quantum Number	Number and Type of Orbitals in the Subshell
Symbol = n Values = 1, 2, 3, . . . n = number of subshells	Symbol = ℓ Values = 0 . . . $n - 1$	Symbol = m_ℓ Values = $+\ell$ . . . 0 . . . $-\ell$	Number of orbitals in shell = n^2 and number of orbitals in subshell = $2\ell + 1$
1	0	0	one 1*s* orbital (one orbital of one type in the $n = 1$ shell)
2	0 1	0 +1, 0, −1	one 2*s* orbital three 2*p* orbitals (four orbitals of two types in the $n = 2$ shell)
3	0 1 2	0 +1, 0, −1 +2, +1, 0, −1, −2	one 3*s* orbital three 3*p* orbitals five 3*d* orbitals (nine orbitals of three types in the $n = 3$ shell)
4	0 1 2 3	0 +1, 0, −1 +2, +1, 0, −1, −2 +3, +2, +1, 0, −1, −2, −3	one 4*s* orbital three 4*p* orbitals five 4*d* orbitals seven 4*f* orbitals (16 orbitals of four types in the $n = 4$ shell)

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❖ **In general**,
- the number of sublevels within a level = *n.*
- the number of orbitals within a sublevel = $2l + 1$.
- the number of orbitals in a level n^2.

� Learning Check

(a) The quantum number n describes the ________ of an atomic orbital, and the quantum number ℓ scribes its ________

(b) When *n* = 3, the possible values of ℓ are ______

(c) What type of orbital corresponds to ℓ = 3? ______

(d) For a *4d* orbital, the value of *n* is _________ , the value of ℓ is ________ , and a possible value of m_l Is ____

(e)There are ____________ orbitals in the third shell.

(f)The principal quantum number of the first d subshell is ____________.

� If an electron has a principal quantum number (n) of 3 and an angular momentum quantum number (ℓ) of 2,
the subshell designation is _________.

� Which one of the following represents an impossible set of quantum numbers for an electron in an atom?
(arranged as n, ℓ , mℓ , and ms)

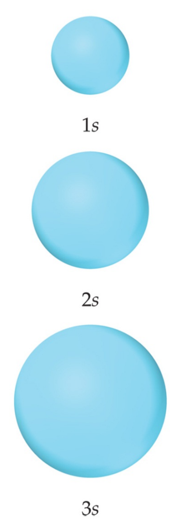
A) 2, 1, -1, -1/2
B) 1, 0, 0, 1/2
C) 3, 3, 3, 1/2
D) 5, 4, - 3, 1/2
E) 5, 4, -3, -1/2

The Shapes of Atomic Orbitals:

- ℓ can have integer values from
  0 to (*n* – 1).

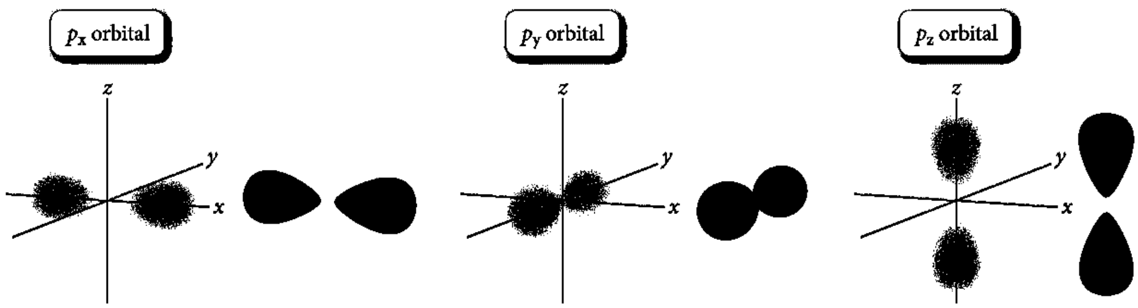
★ **ℓ = 0, the *s* Orbital**

- They are spherical in shape.
- The radius of the sphere increases with the value of *n.*
- *As n increases, the number of nodes increases.*
- Number of nodes = (*n* – 1)



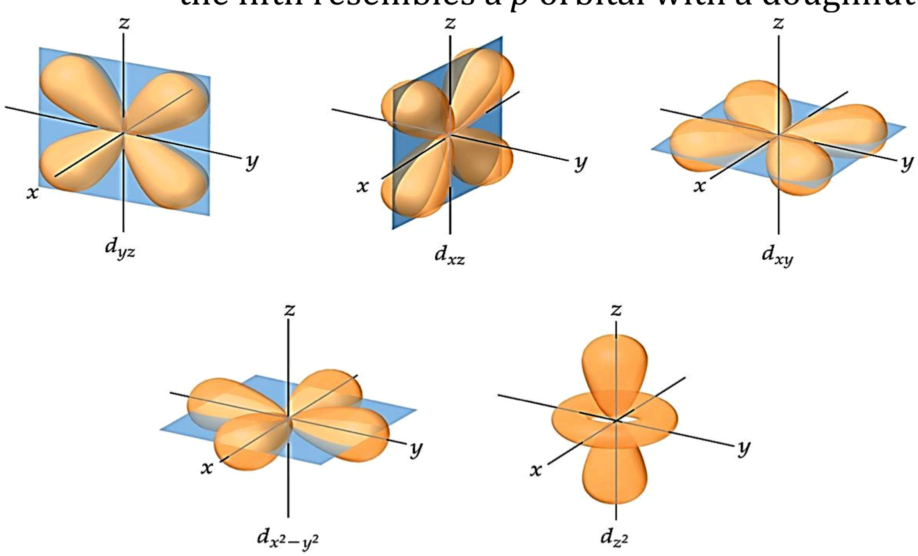
ℓ = 1, *p* orbitals

- All p orbitals have two lobes with a node between them (at the nucleus)
- • There are three *p* orbitals: p_x, p_y, and p_z.
- • The letters correspond to allowed values of m_l of −1, 0, and +1.
- • As *n* increases, the *p* orbitals get larger.



ℓ = 2, *d* Orbitals

- The value of ℓ for a *d* orbital is 2.
- Four of the five *d* orbitals have 4 lobes;
- the fifth resembles a *p* orbital with a doughnut around the center.



The value of ℓ for a *f* orbital is 3.
7 possible f orbitals.