# Atomic Structure

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# Atomic Structure

Atoms are made up of 3 types of particles **electrons**  , **protons**  and **neutrons**  . These particles have different properties. **Electrons** are tiny, very light particles that have a negative electrical charge (-). **Protons** are much larger and heavier than electrons and have the opposite charge, protons have a positive charge. **Neutrons** are large and heavy like protons, however neutrons have no electrical charge. Each atom is made up of a combination of these particles.

Electrons revolve around the nucleus in different energy levels or shells

and each shell is having a definite energy

The energy of the K shell is the least

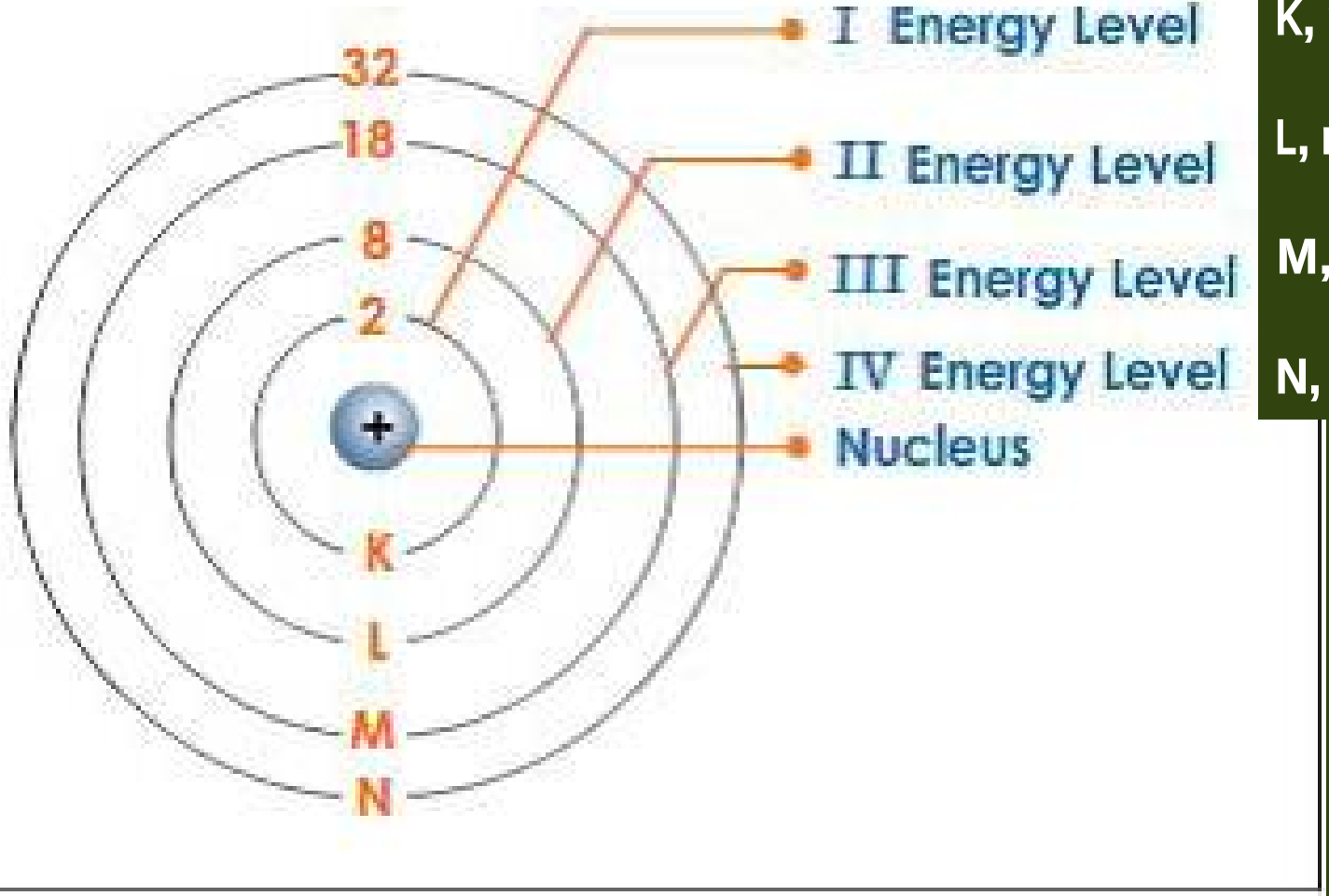
while those of L, M, N and O shells increases.

1st energy level is K shell, 2nd energy level is L shell,

3rd energy level is M shell,

and 4th energy level is N shell .....and so on.....

- X




K, n=1

L, n=2

M, n=3

N, n=4

**Maximum number of electrons** that can be accommodated in a shell is given by **$2n^2$** Where **n = shell number**

**Maximum number of electrons in K energy level = $2n^2$ =2 x $(1)^2$ = 2**

**L energy level , n = 2,**

- **Maximum number of electrons in L energy level = $2n^2$ =2 x $2^2$ = 2 x 4 = 8**

**M energy level, n = 3,**

**Maximum number of electrons in M energy level = $2n^2$ = 2 x $(3)^2$ = 2 x 9 = 18**

**N energy level, n = 4,**

**Maximum number of electrons in N energy level = $2n^2$ = 2 x $(4)^2$ = 2 x 16 = 32 And so on.....**

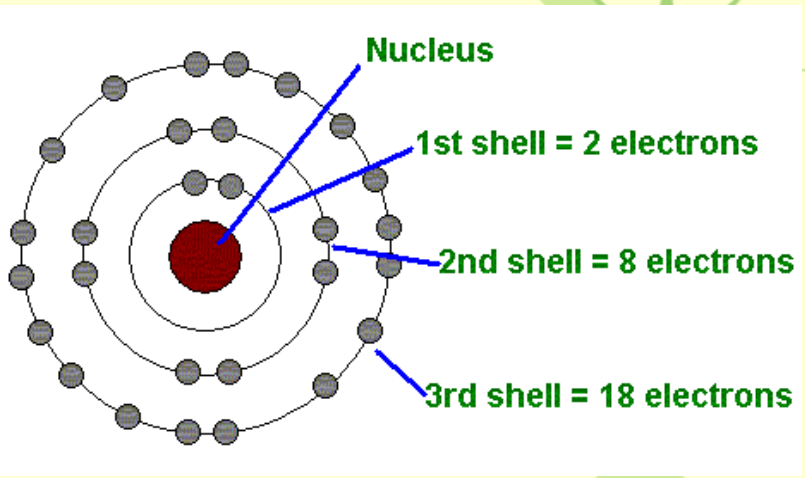
- **Rule: The outermost shell of an atom cannot fill more than 8 electrons, even if it has a capacity to fill more electrons. This is called the Octet rule.**

# Atomic Structure

**The electrons are arranged in Energy levels or "SHELLS" around the nucleus of an atom.**

**Shells can contain a certain maximum number of electrons**

**Shell with the lowest energy fills first**




**The maximum number of electrons** in each shell can be given by formula $2n^2$

| **Shell number** | **1** | **2** | **3** | **4** |
|---|---|---|---|---|
| **Formula $2n^2$** | **$2(1)^2$** | **$2(2)^2$** | **$2(3)^2$** | **$2(4)^2$** |
| **Maximum number of electrons** | **2** | **8** | **18** | **32** |

| Element | Symbol | Atomic number | Electronic configuration (or Electron arrangement) K L M N |
|---|---|---|---|
| Hydrogen | H | 1 | 1 |
| Helium | He | 2 | 2 |
| Lithium | Li | 3 | 2,1 |
| Beryllium | Be | 4 | 2,2 |
| Boron | B | 5 | 2,3 |
| Carbon | C | 6 | 2,4 |
| Nitrogen | N | 7 | 2,5 |
| Oxygen | O | 8 | 2,6 |
| Fluorine | F | 9 | 2,7 |
| Neon | Ne | 10 | 2,8 |

- 
- 

| Element | Symbol | Atomic number | Electronic configuration (or Electron arrangement) K L M N |
|---|---|---|---|
| Sodium | Na | 11 | 2,8,1 |
| Magnesium | Mg | 12 | 2,8,2 |
| Aluminum | Al | 13 | 2,8,3 |
| Silicon | Si | 14 | 2,8,4 |
| Phosphorus | P | 15 | 2,8,5 |
| Sulphur | S | 16 | 2,8,6 |
| Chlorine | Cl | 17 | 2,8,7 |
| Argon | Ar | 18 | 2,8,8 |
| Potassium | K | 19 | 2,8,8,1 |
| Calcium | Ca | 20 | 2,8,8,2 |

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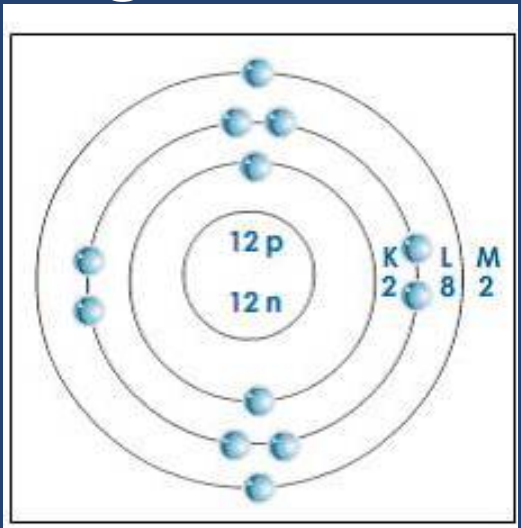
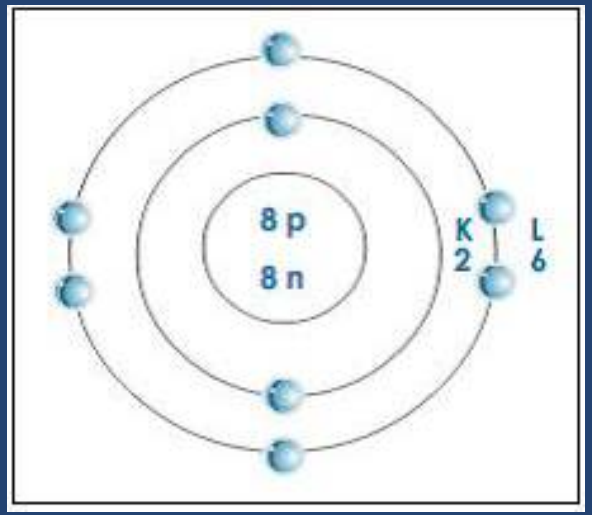
- 

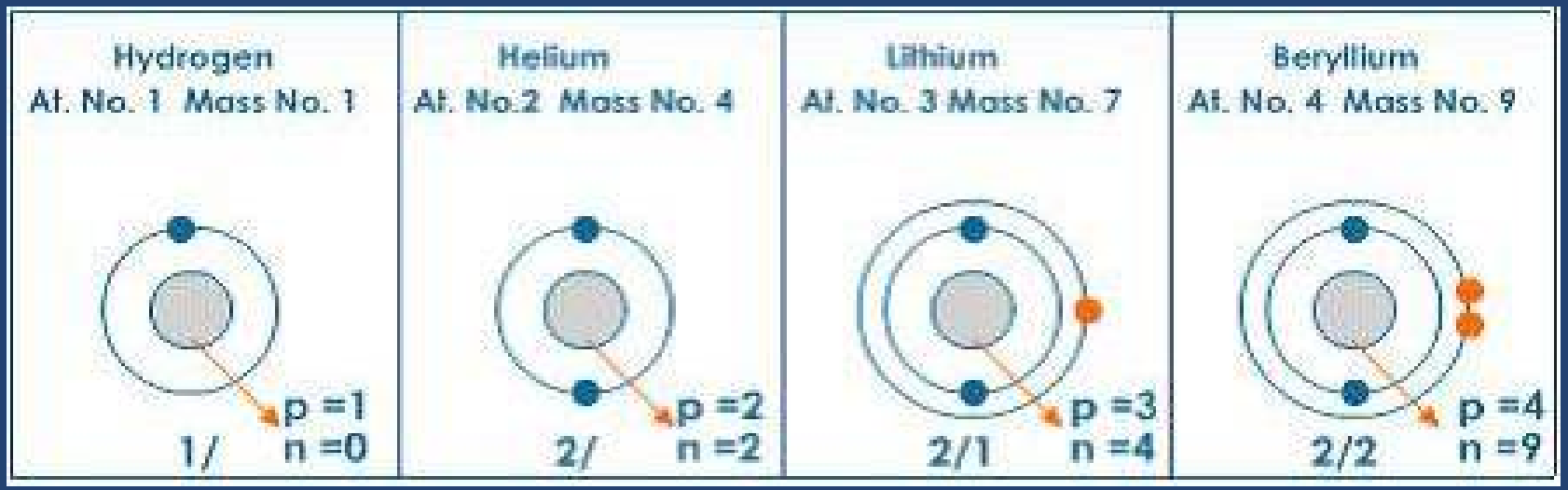
# Diagrammatic Representation of Atomic Structure:

## Magnesium-12

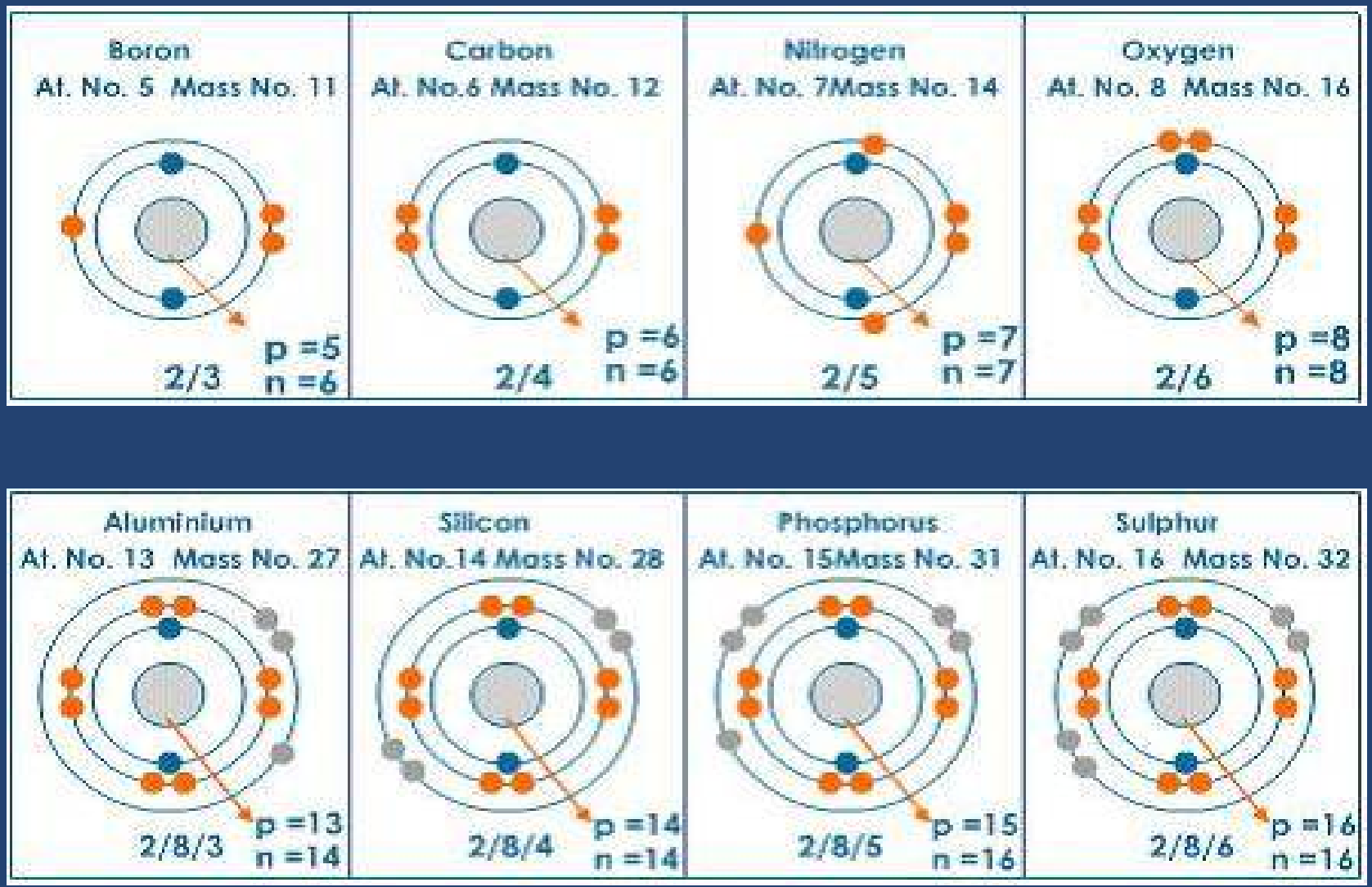



## Oxygen-8



# Diagrammatic Representation of Atomic Structure:



# Electronic Configuration of the Element:

The electron configuration of an atom is a form of notation which shows how the electrons are distributed among the various atomic orbital and energy levels.

$1s^2$

**The number "1" refers to the principle quantum number "n" which stands for the energy level**

**The letter "s" stands for the angular quantum number "l".**

**For a given value of n, l can have n values ranging from 0 to (n – 1),**

**that is, for a given value of n, the possible values of l are:**

**l= 0, 1, 2..... (n – 1)**

**For example, when n=1, value of l is only 0.**

**For n=2, the possible value of l can be 0 and 1.**

**For n=3, the possible l values are 0, 1 and 2**

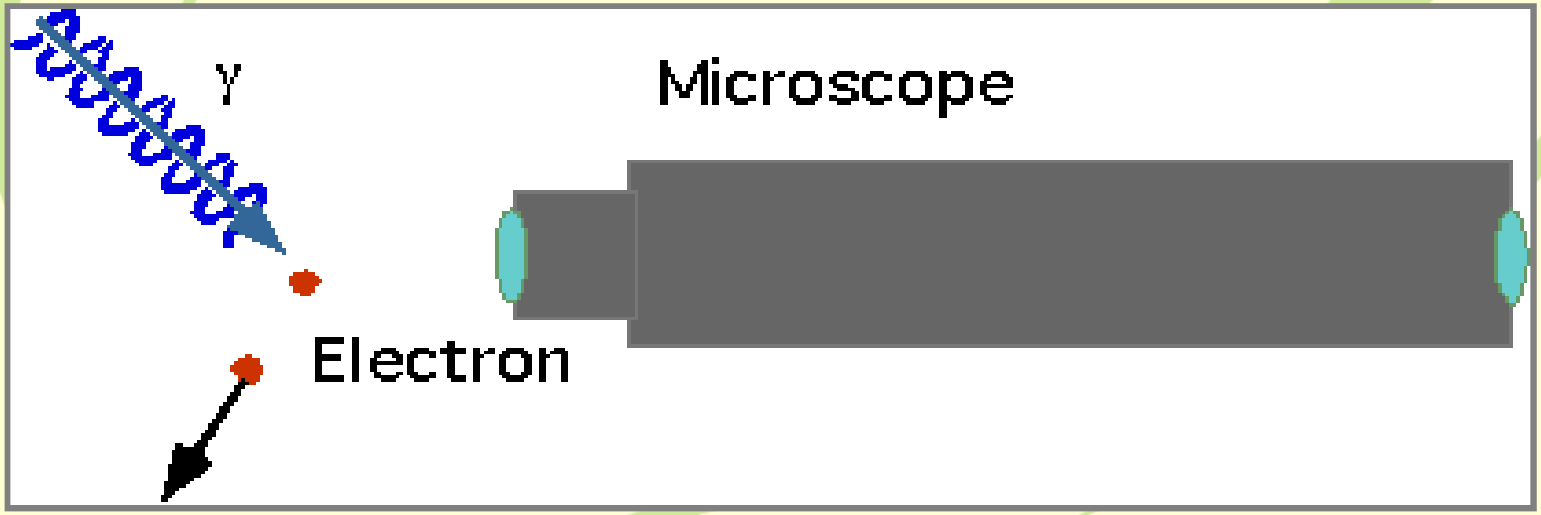
# The Heisenburg uncertainty principle

The photon particle travels at approximately the same velocity as the electron particle, so that…….

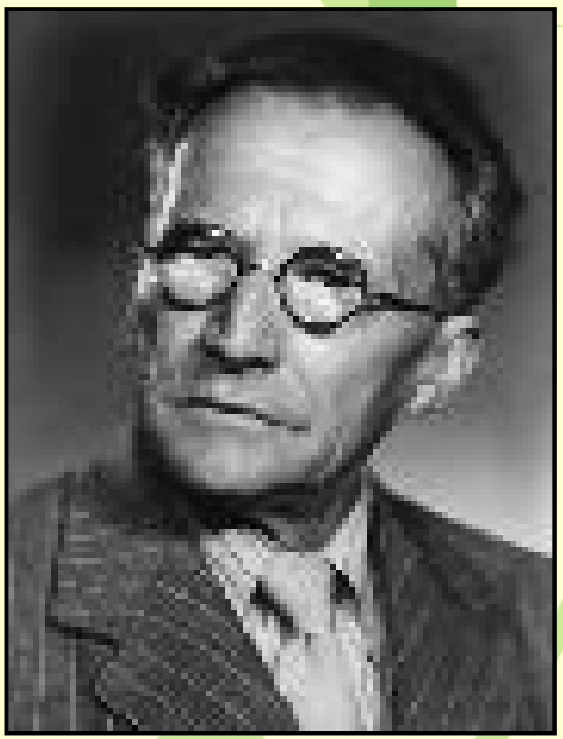
The photon particle travels at approximately the same velocity as the electron particle, so that…… when it impacts the electron it alters its position as when two asteroids collide into each other at similar velocities but different angles.

Therefore, according to Heisenburg,

***it is impossible to know decisively an electron's position and momentum.***



# The Schrödinger Wave Equation



- **Schrödinger** applied **de Broglie's** concept of matter waves to the electron

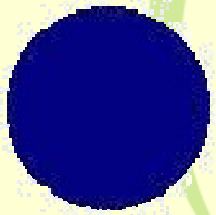
- He provided a **mathematical equation (wave function)** to describe electron waves and determine the **PROBABILITY** of where that electron is in the atom (remember Heisenberg...)

- These regions of probability are called **orbitals,** and this concept replaces that of the electron "orbit".

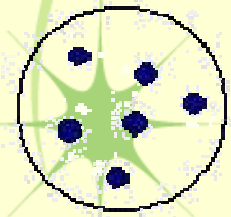
# Schrodinger Wave Equation, contd.

- Instead of electrons orbiting like planets around the sun, **Schrodinger's picture shows an "electron cloud" surrounding the nucleus** and doesn't state anything about the path or position of electrons within that cloud.

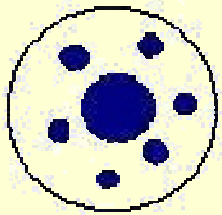
- Orbital "pictures" shown in texts represent regions of space where the probability of finding an electron **is 90% or greater**.



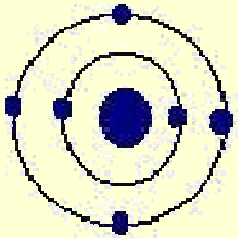
a. Dalton's model



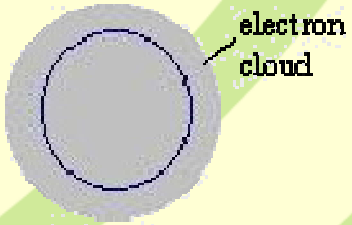
b. Thomson's model



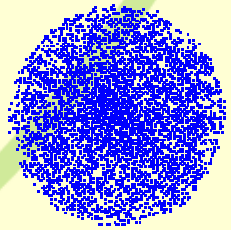
c. Rutherford's model



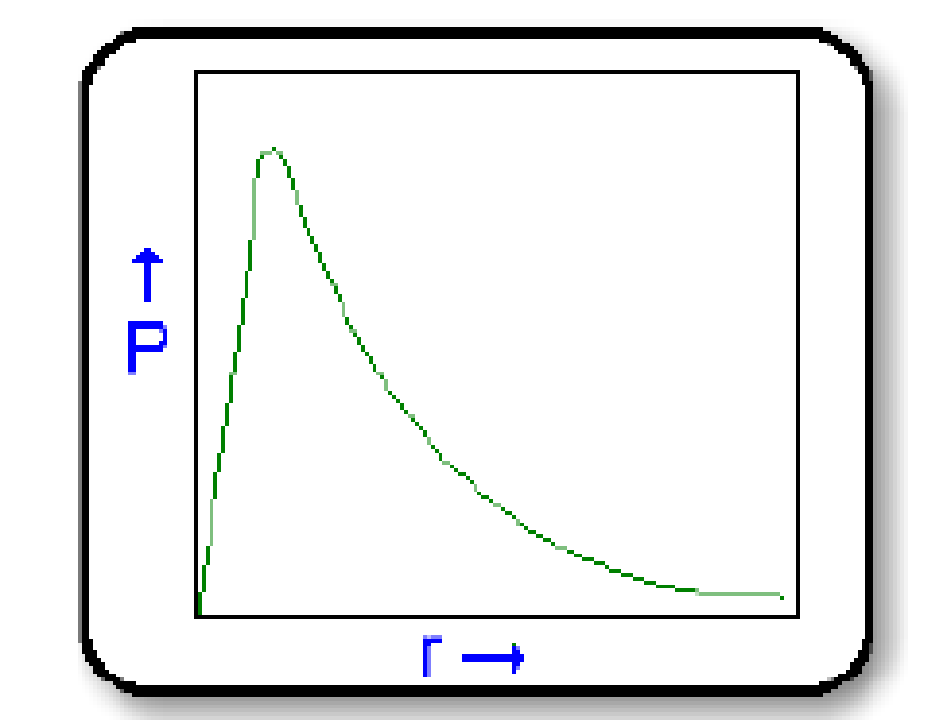
d. Bohr's model

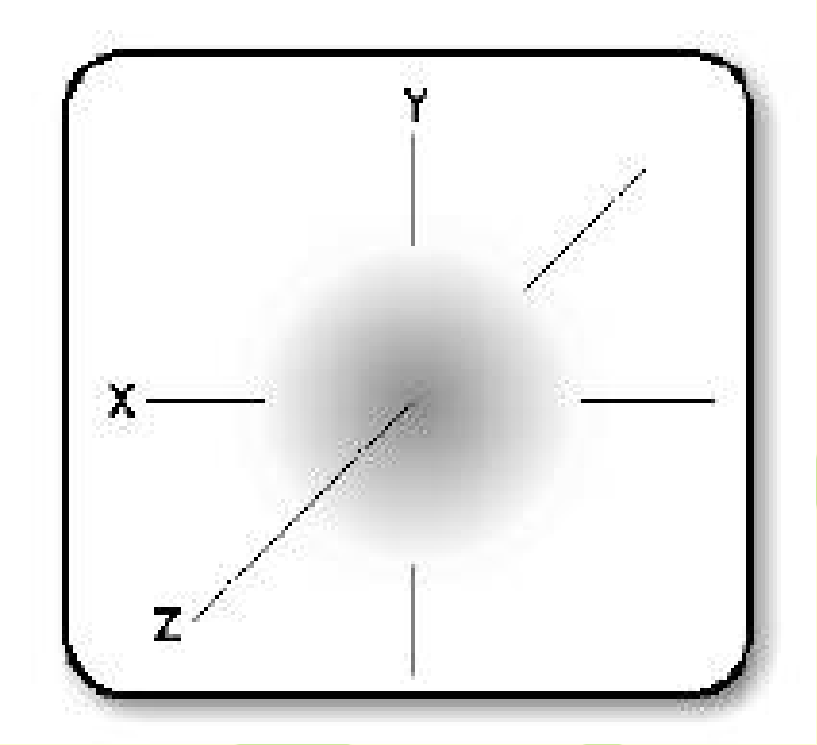



e. Quantum mechanical model



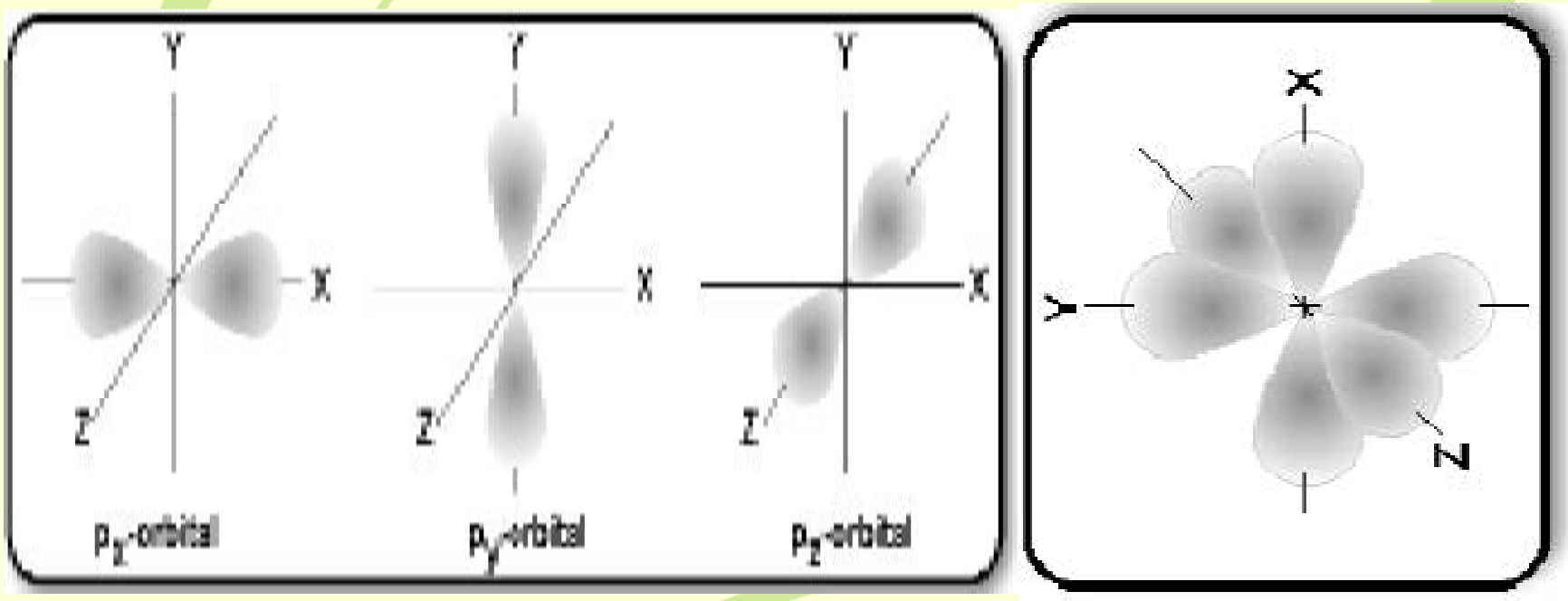
# 1. S-like Atomic Orbitals



# *p-like Atomic Orbitals*

•p-Orbitals consist of **electron clouds** which look like the diagram on the right, with a node at the nucleus of the atom. There are three such orbitals, oriented at right angles to one another, as shown in the diagram below:



# Quantum Numbers

- Schrodinger's wave equation used 4 **quantum numbers** to describe the size & energy, shape, and orientations of the orbitals in atoms.

- This set of four numbers provides us with an **"orbital address"** for an electron within an atom – we can describe the orbital in which an electron is found if we know these three quantum numbers.

# Quantum Numbers

Each electron in an atom has a unique set of 4 quantum numbers which describe it.

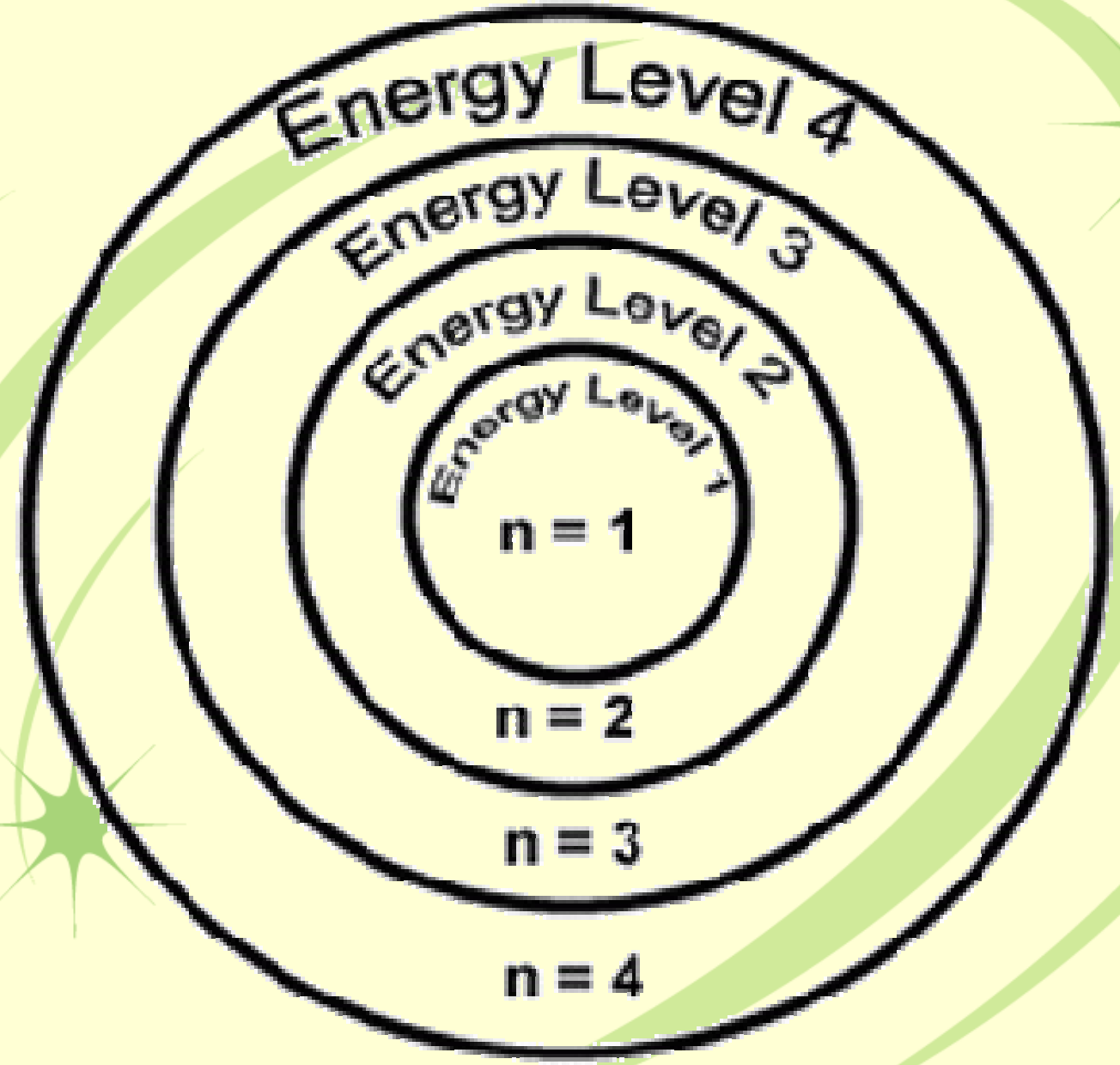
- Principal quantum number ***n,***
- Angular momentum quantum number ***l ,***
- Magnetic quantum number $m_l$,
- Spin quantum number $m_s$

# Principal Quantum Number, n

- n can have values **≥ 1, integers** only.
- As n increases, energy of electron and size of energy level increases.
- Larger n means greater probability of greater distance from the nucleus.

n can only be integers starting from 1.

n= 1, 2, 3, 4, ....


Energy Level 4
Energy Level 3
Energy Level 2
Energy Level 1
n = 1
n = 2
n = 3
n = 4

# Angular Quantum Number, **l** (Shape)

- The values for **l** (lower case letter L, script) are limited by the principal energy level – they range from **0 to "n–1"**

- Example:

If **n = 1,** **l** can be 0 (s ) [K]

If **n = 2,** **l** can be 0 , 1 ( s,p) [L]

If **n = 3,** **l** can be 0, 1 , 2 (s,p,d) [M]

# Angular Quantum Number, *l*

## More about the 2nd Quantum # *l*

- ***l* gives information about <u>shape</u> of orbital**

| | |
|---|---|
| ***l* = 0** | ***(found on all principle energy levels)*** |
| ***l* = 1** | ***(found on level 2 and higher)*** |
| ***l* = 2** | ***(found on level 3 and higher)*** |
| ***l* = 3** | ***(found on level 4 and higher)*** |

# Azimuthal Quantum Number, $m_l$

## Magnetic Quantum Number

This **tells you the orientation** of the shape in the 3 dimensional axis

$m_l = -l,.., 0, ...l$

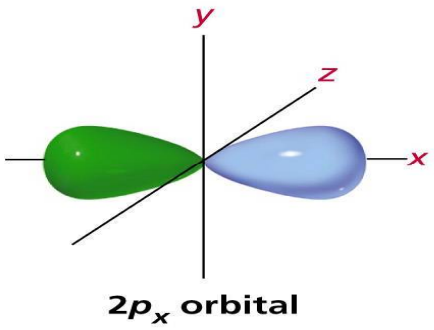
So **if** $l = 1$, there are **3 possibilities for** $m_l$

These are: **-1,0,1**

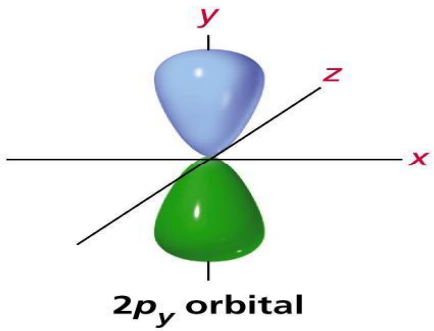
# Third Quantum # $m_l$ (continued)

....There are **3 possibilities for the orientation of this shape.**

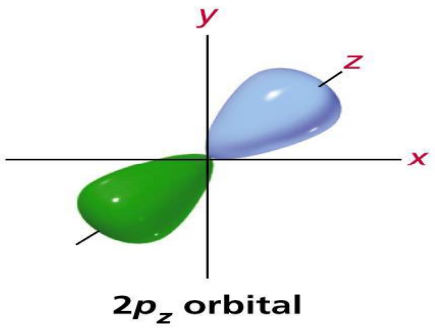
- Since **we are in 3dimensional space,** we must have **3 axis: x, y, z.** All orbitals exist in this space.



$2p_x$ orbital



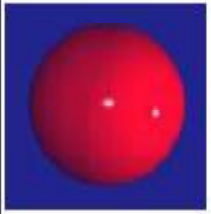
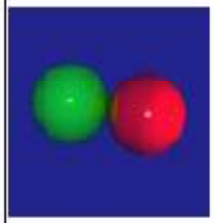
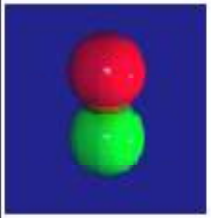
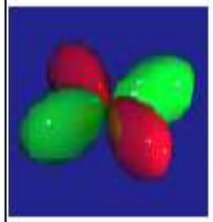
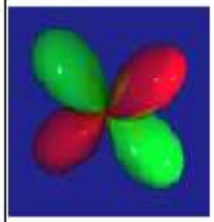
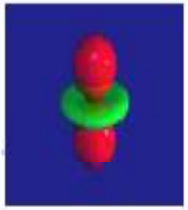
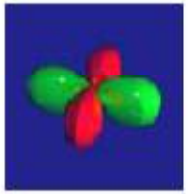
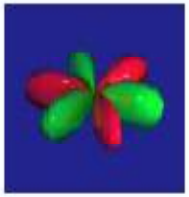
$2p_y$ orbital



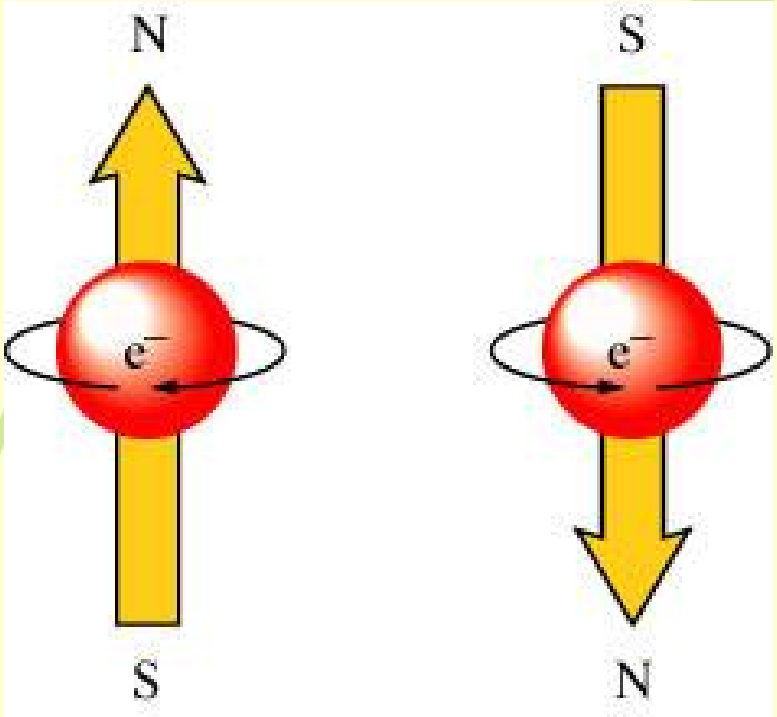
$2p_z$ orbital

$m_l$

$l$

| | -3 | -2 | -1 | ml=0 | 1 | 2 | 3 |
|---|---|---|---|---|---|---|---|
| l–0 | | | |  | | | |
| l=1 | | |  |  |  | | |
| l=2 | |  |  |  |  |  | |
| l=3 |  |  |  |  |  |  |  |

# Electron Spin Quantum Number, $m_s$




A fourth quantum number, $m_s$ describes **electron spin** (either $+\frac{1}{2}$ or $-\frac{1}{2}$)

This allows a maximum of 2 electrons per orbital.

*A spinning negative charge creates a magnetic field. The direction of spin d determines the direction of the field.*

# Putting it Together...

- Electrons with the same **n** value are said to be in the same **energy level** or **shell**.
- Electrons with same **n and l** values are said to be in the same **subshell.**
- Electrons with the same, **n, l , and $m_l$**, are in the same **orbital**.
- There are a maximum of **2 electrons** (+1/2 & -1/2) **in each orbital**.

## Quantum numbers for the first four levels of orbitals in the hydrogen atom

| n | l | Orbital designation | $m_l$ | # of orbitals |
|---|---|---|---|---|
| 1 | 0 | 1s | 0 | 1 |
| 2 | 0 | 2s | 0 | 1 |
| | 1 | 2p | -1, 0, 1 | 3 |
| 3 | 0 | 3s | 0 | 1 |
| | 1 | 3p | -1, 0, 1 | 3 |
| | 2 | 3d | -2, -1, 0, 1, 2 | 5 |
| 4 | 0 | 4s | 0 | 1 |
| | 1 | 4p | -1, 0, 1 | 3 |
| | 2 | 4d | -2, -1, 0, 1, 2 | 5 |
| | 3 | 4f | -3, -2, -1, 0, 1, 2, 3 | 7 |

Each shell consists of one or more **subshell**s or **sub- levels.** The number of subshells in a principal shell is equal to the value of n. for example

in the **first shell (n=1),** there is **only one sub-shell** which corresponds to **l=0.**

There are **two sub-shells (l=0, 1)** in the second shell **(n=2),**

**three (l=0, 1, 2)** in **third shell (n=3)** and so on.

Each sub-shell is assigned an angular quantum number (l). represented by the following symbols.

**Value for l:** 0 1 2 3 4 5.....

**Sub- shell: s p d f g h.....**

• The exponent "2" refers to the total number of electrons in that orbital or sub-shell.

# Principle Quantum Number (n) and Sublevels

The number of sublevels that an energy level can contain is equal to the principle quantum number of that level.
So, for example,

the **second energy** level would have **two sublevels,** and the

**third** energy level would have **three sublevels.**

***The first sublevel is called an s sublevel.***

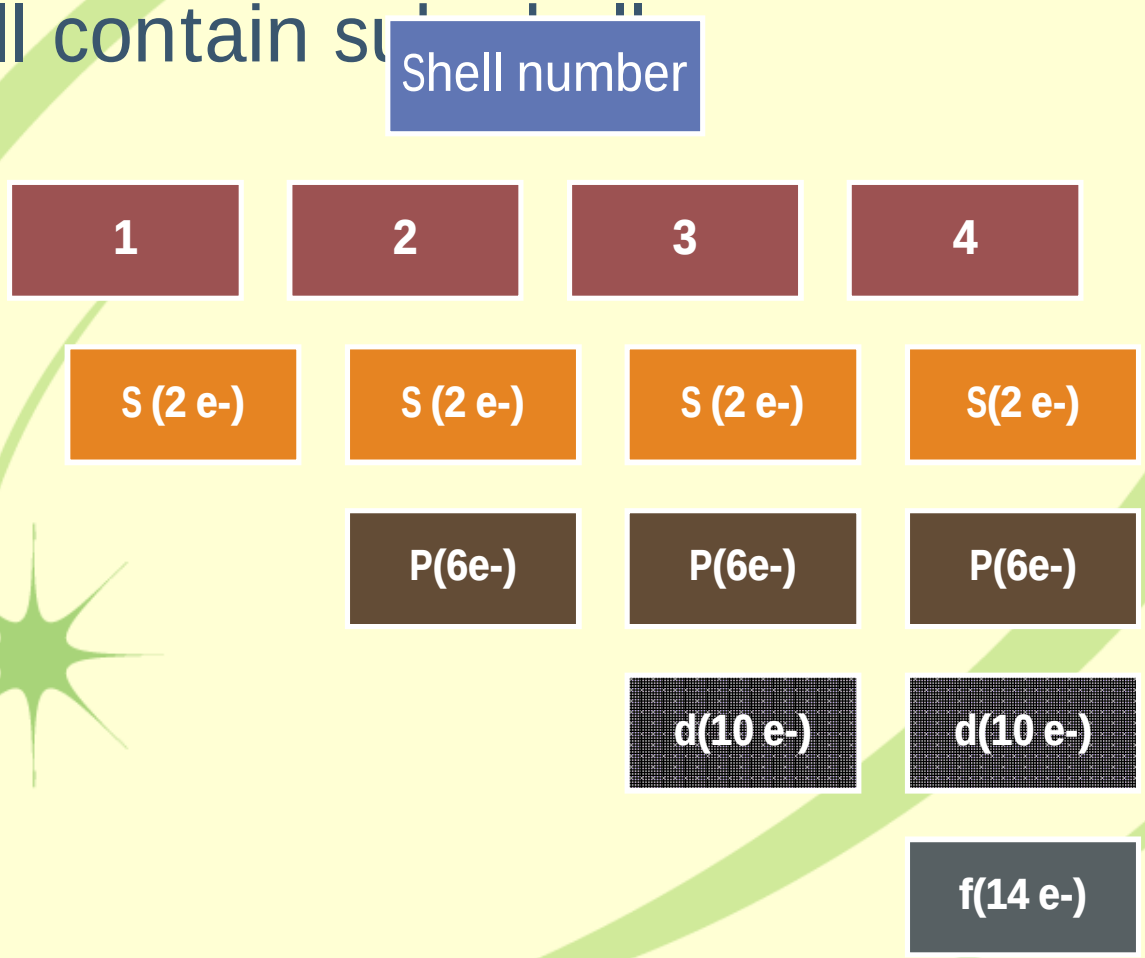
***The second sublevel is called a p sublevel.***

***The third sublevel is called a d sublevel and the fourth sublevel is called an f sublevel.***

# Electronic Configuration

Electronic configuration: shows how electrons arranged in shells by indicating the number of electrons in their shells and number of shells.

Each shell contain su

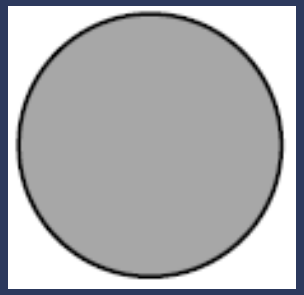


## II. Sublevels and

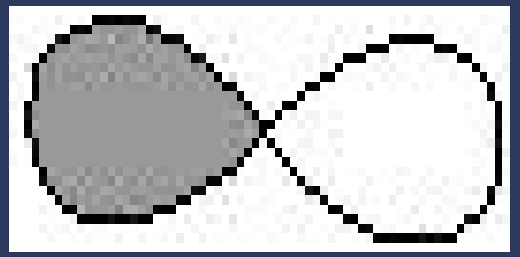
An orbital is a space that **can be occupied by up to two electrons**. Each type of **sublevel holds a different number of Orbital,** and therefore, a different number of electrons.

| Sublevel | No. of Orbitals | Maximum number of electrons |
|---|---|---|
| s | 1 | 2 |
| p | 3 | 6 |
| d | 5 | 10 |
| f | 7 | 14 |

- **Shapes of the orbital:**



**s- Orbital**



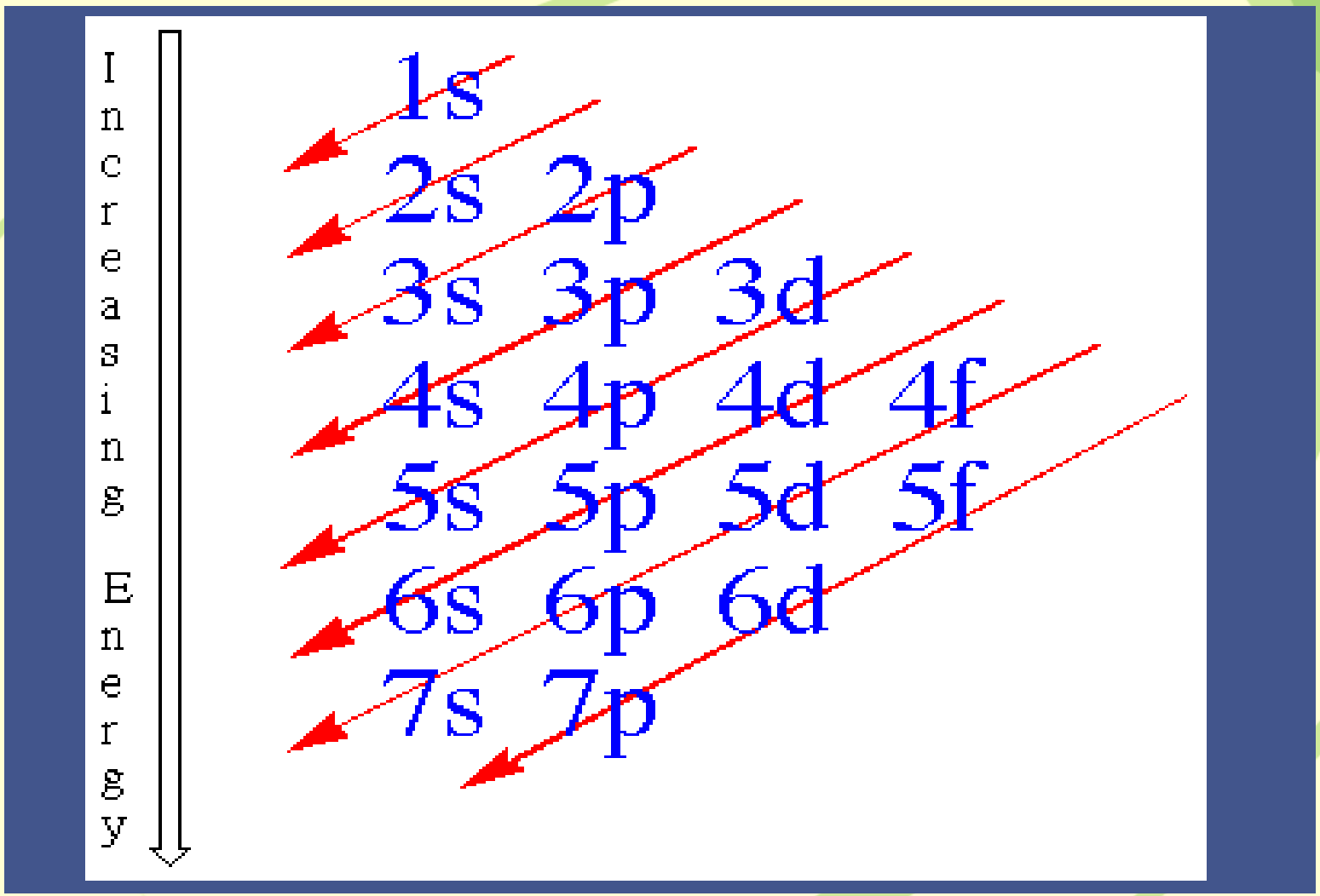
**p- Orbital**

**Spherical** **Dumbbell**

# IV. **Total Number of Electrons per Energy Level**

| Principle energy level (n) | Type of sublevel | Number of Orbitals per type | Number of Orbitals per level($n^2$) | Maximum number of electrons ($2n^2$) |
|---|---|---|---|---|
| 1 | s | 1 | 1 | 2 |
| 2 | s | 1 | 4 | 8 |
| | p | 3 | | |
| 3 | s | 1 | 9 | 18 |
| | p | 3 | | |
| | d | 5 | | |
| 4 | s | 1 | 16 | 32 |
| | p | 3 | | |
| | d | 5 | | |
| | f | 7 | | |

# IV. Order of Filling Sublevels with Electrons



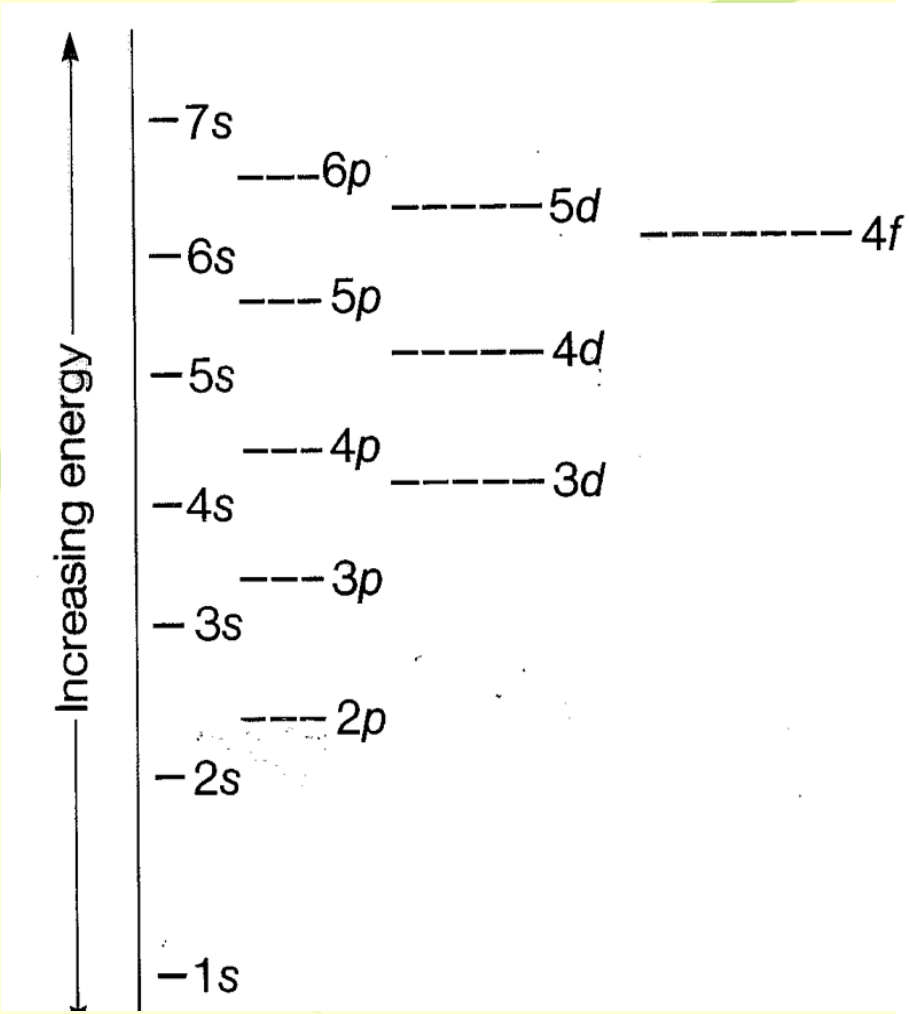

**The order for filling in the sublevels ;**
**1s, 2s, 2p, 3s, 3p, 4s, 3d, 4p, 5s, 4d, 5p, 6s, 4f, 5d, 6p, 7s, 5f, 6d,7p.**

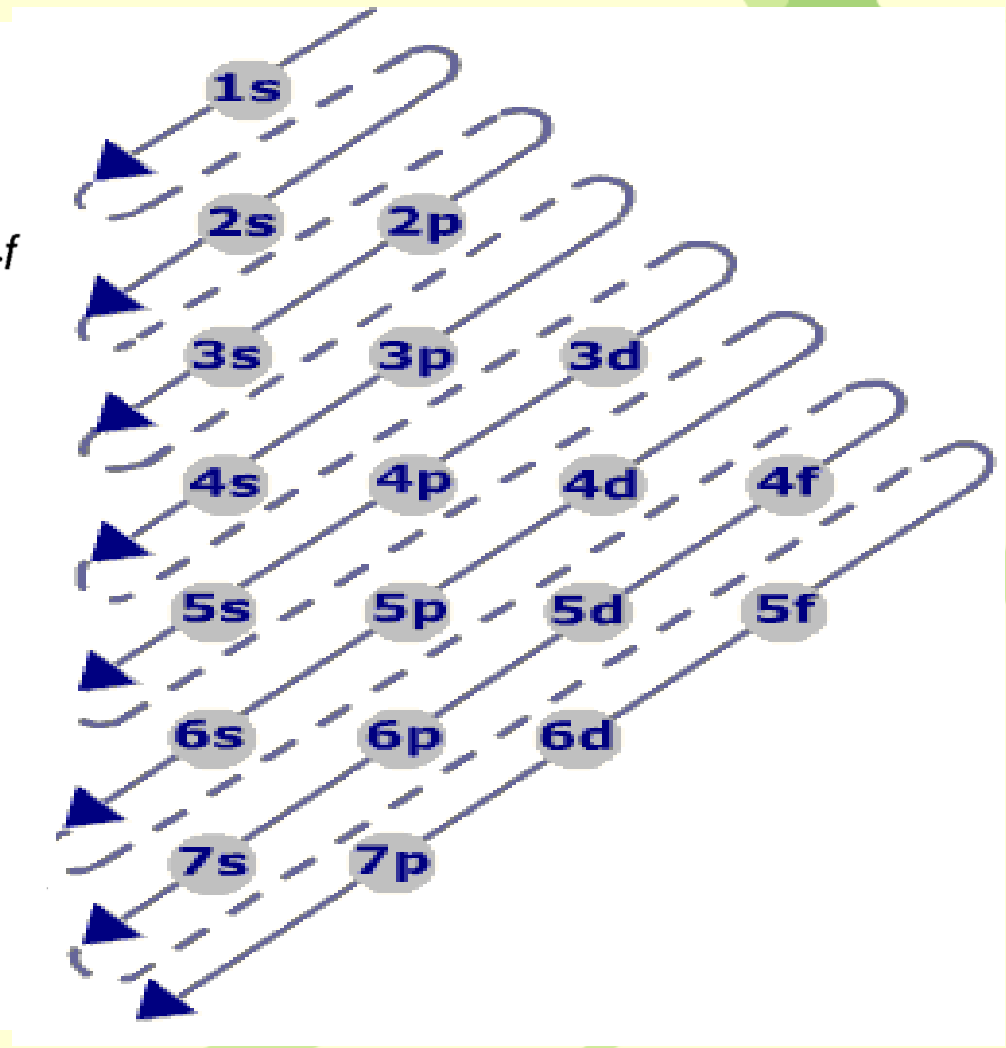
# Rules of writing the Electronic Configuration:

states no two electrons within a particular atom can have identical quantum numbers.

states that when more than one orbital of equal energies are available then the electrons will first occupy these orbitals separately with parallel spins.

# Electronic Configuration : Aufbau Principle



# Electronic Configuration : Aufbau Principle

**$Na^+$ & $O^{2-}$ have same electronic configuration as Ne :$1s^2\ 2s^2\ 2p^6$**

**So they are isoelctronic with Ne**

Example :What is the electron configuration of Na, Ca, Fe & O and their corresponding ions?

- **Na:**
  **$1s^2\ 2s^2\ 2p^6\ 3s^1$**
- **O:**
  **$1s^2\ 2s^2\ 2p^4$**
- **Ca:**
  **$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2$**
- **Fe:**
  **$1s^2\ 2s^2\ 2p^6\ 3S^2\ 3p^6\ 4S^2\ 3d^6$**

- **$Na^+$:**
  **$1s^2\ 2s^2\ 2p^6$**
- **$O^{2-}$:**
  **$1s^2\ 2s^2\ 2p^6$**
- **$Ca^{2+}$:**
  **$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6$**
- **$Fe^{2+}$:**
  **$1s^2\ 2s^2\ 2p^4\ 3S^2\ 3p^6\ 3d^6$**

# Electronic Configuration : Aufbau Principle

Do yourself: Write the electron configuration using s, p, d and f **notations** of the following atoms:

a. Cl

b. Mg

c. F

d. $N^{3-}$

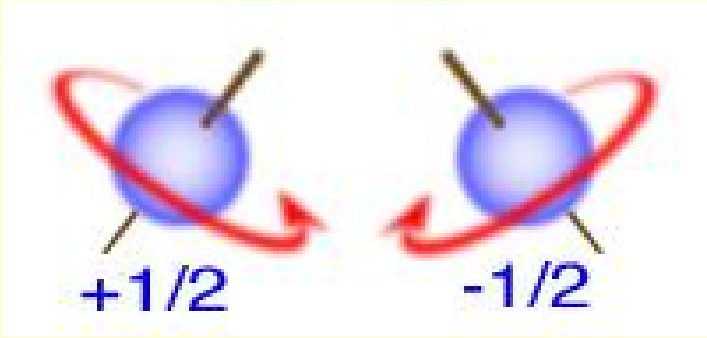
f. $K^{+}$

e. $Ti^{4+}$

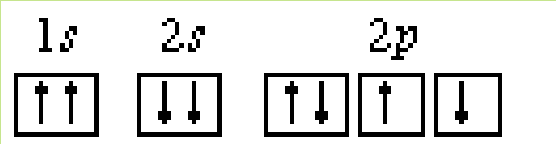
# Rules of writing the Electronic Configuration:

states that electrons always fill orbital of lower energy first.
Example: **1*s* is filled before 2*s*, and 2*s* before 2*p*.**

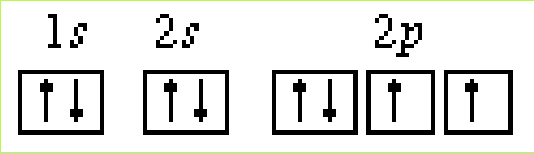
states no two electrons within a particular atom can have identical quantum numbers.




When we draw electrons, we use up and down arrows. **So, if an electron is paired up in a box, one arrow is up and the second must be down.**




**Incorrect**; electrons must spin in opposite directions




**Correct; the electrons have opposite spins**

# Rules of writing the Electronic Configuration:

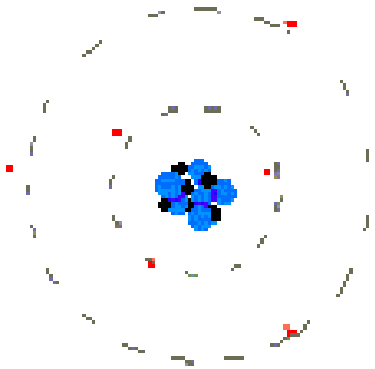
states that when more than one orbital of equal energies are available then the electrons will first occupy these orbitals separately with parallel spins.

The pairing of electrons will start only after all the orbital of a given sub level are singly occupied.

Example: 3 electrons that are filled into the three 'p' orbital can be represented in two different ways:

## This Atom is Neutral

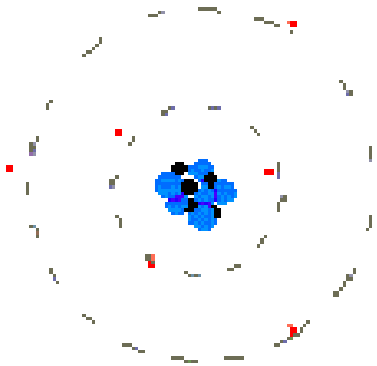
*Same number of protons and electrons*



- 6 Protons
- 6 Neutrons
- 6 Electrons

## This Atom is Negatively Charged

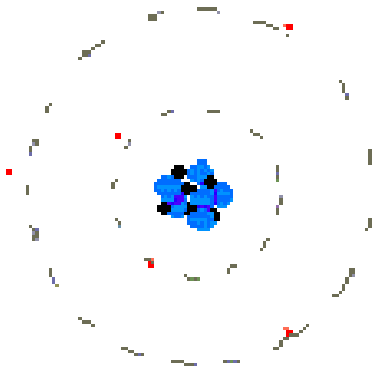
*More electrons than protons*



- 5 Protons
- 6 Neutrons
- 6 Electrons

## This Atom is Positively Charged

*More protons than electrons*



- 6 Protons
- 6 Neutrons
- 5 Electrons

## Electronic Configurations of Ions:

- When we write the electron configuration of a **positive ion**, we **remove** one electron for each positive charge:
- When we write the electron configuration of a **negative ion**, we **add one electron** for each negative charge:

# Electronic Configurations of Ions:

- When we write the electron configuration of a **positive ion**, we **remove** one electron for each positive charge:

$$\begin{array}{ccc} \mathrm{Na} & \rightarrow & \mathrm{Na^+} \\ 1s^2\,2s^2\,2p^6\,3s^1 & \rightarrow & 1s^2\,2s^2\,2p^6 \end{array}$$

- When we write the electron configuration of a **negative ion**, we **add one electron** for each negative charge:

$$\begin{array}{ccc} \mathrm{O} & \rightarrow & \mathrm{O^{2-}} \\ 1s^2\,2s^2\,2p^4 & \rightarrow & 1s^2\,2s^2\,2p^6 \end{array}$$

# Atomic Structure

Reference Books

Solomons & Fryhle, ORGANIC CHEMISTRY,

Wiley. Sykes, A PRIMER TO MECHANISM IN ORGANIC CHEMISTRY,.