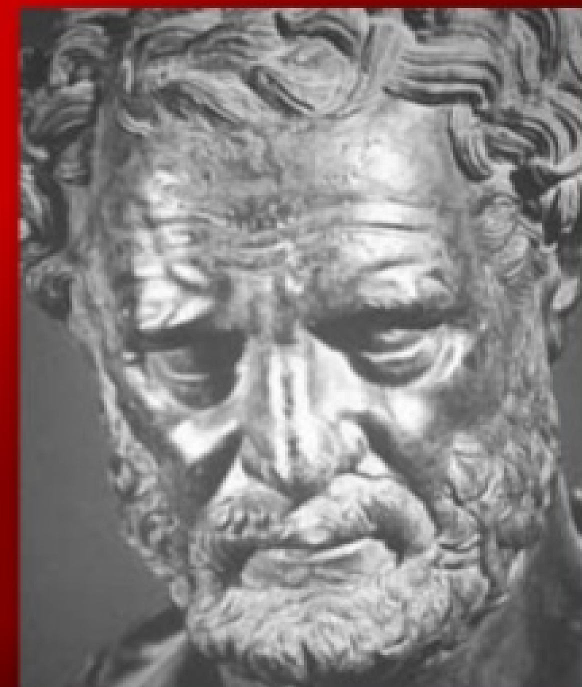
Inorganic Chemistry

- Atomic structure and the periodic table
- Chemical Bonds – ionic, covalent (and hydrogen)
- Chemical elements and substances
- Oxidative-reductive properties
- Velocity
- Solutions, electrolytes

Atomic structure

HISTORY OF THE ATOM

460 BC Democritus develops the idea of atoms



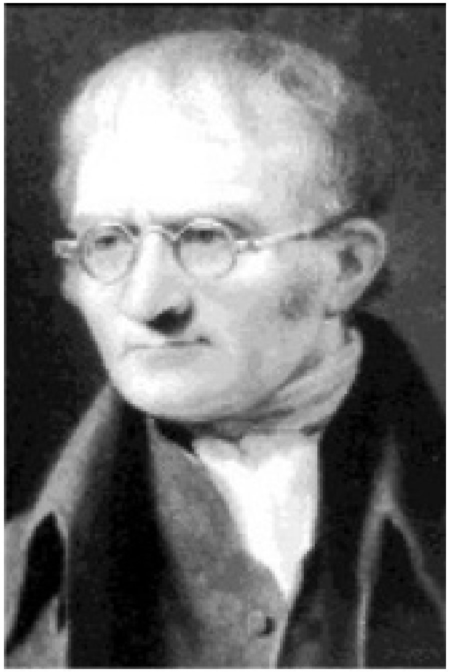
he pounded up materials in his pestle and mortar until he had reduced them to smaller and smaller particles which he called

ATOMA

History of the atom

Atomic Theory

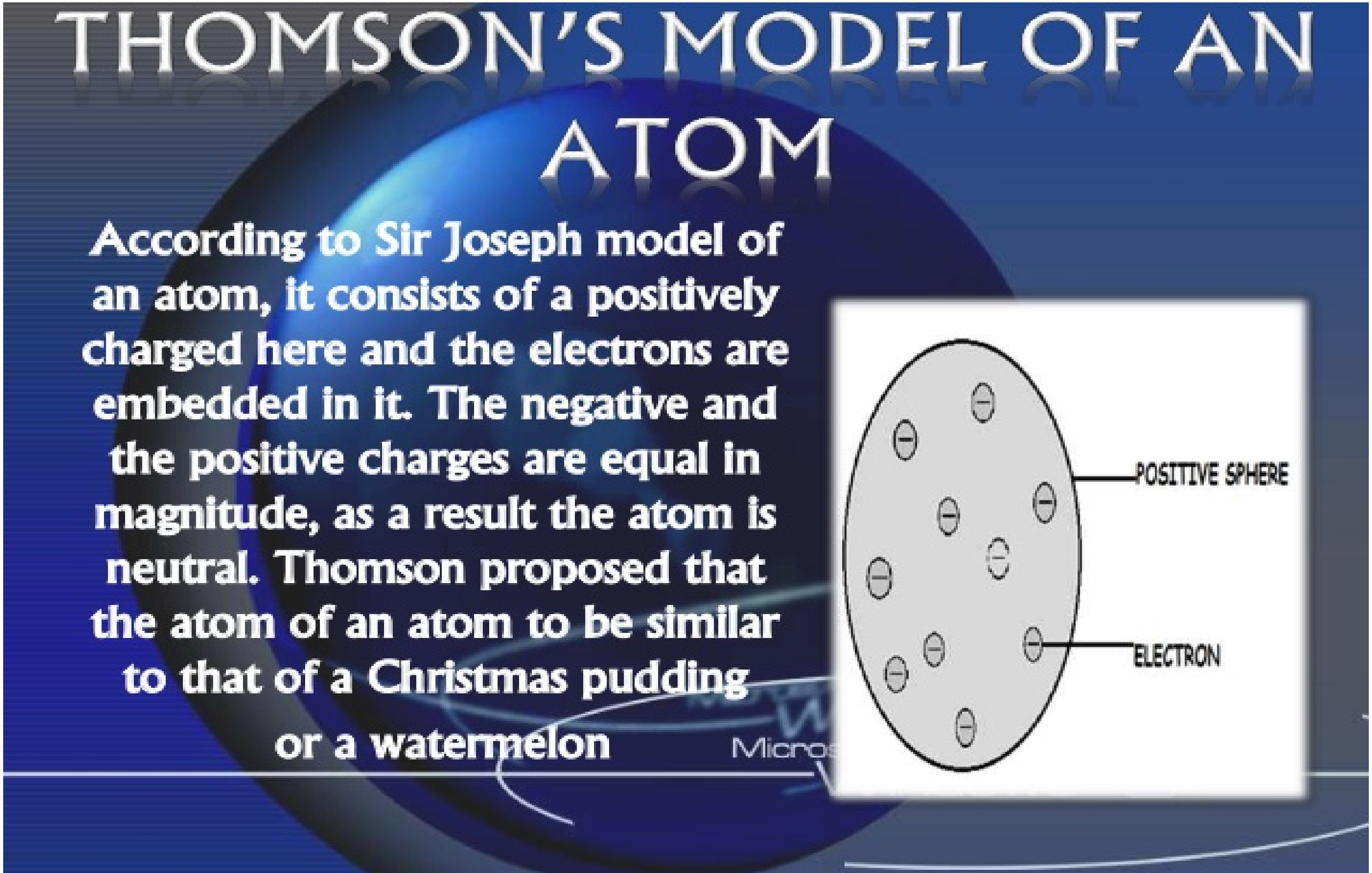
- All matter is made up of atoms.
- Atoms of an element are identical.
- Each element has different atoms.
- Atoms can engage in a chemical reactions.
- Atoms can neither be created nor be destroyed.
- Atoms are indivisible.



John Dalton

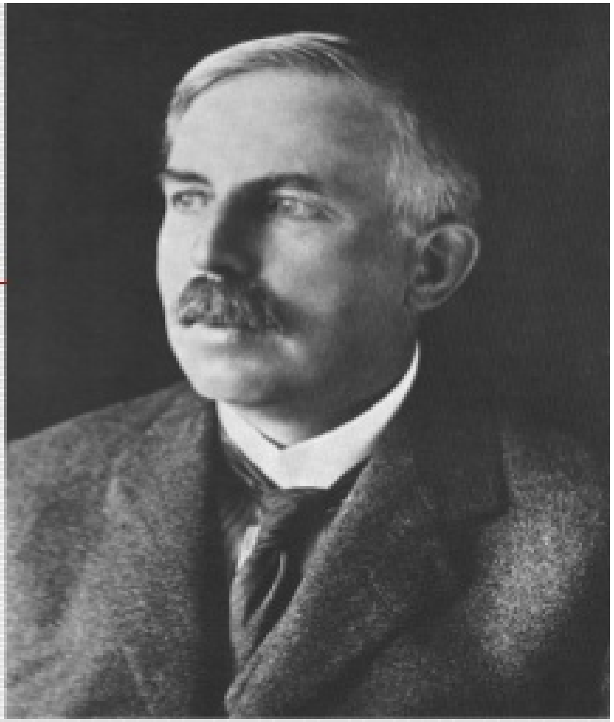
(1776-1884)

History of the atom

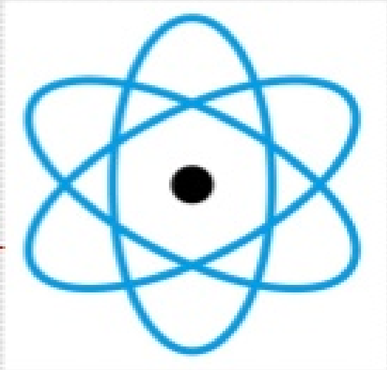


Rutherford's Atomic Model

- atom has a positively charged central part (nucleus)
- Electrons are distributed around nucleus
- Mass of an atom is concentrated at nucleus.
- Compared with total volume of an atom, the volume of nucleus is meager

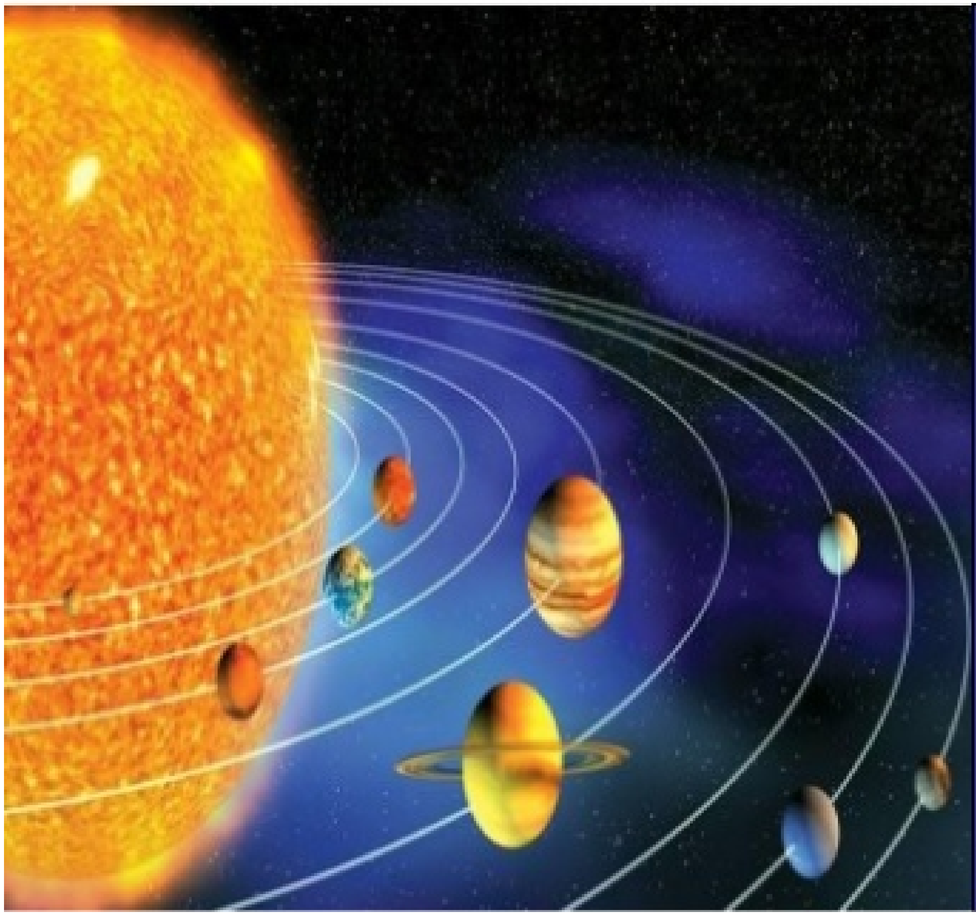


Ernest Rutherford
(1871-1937)

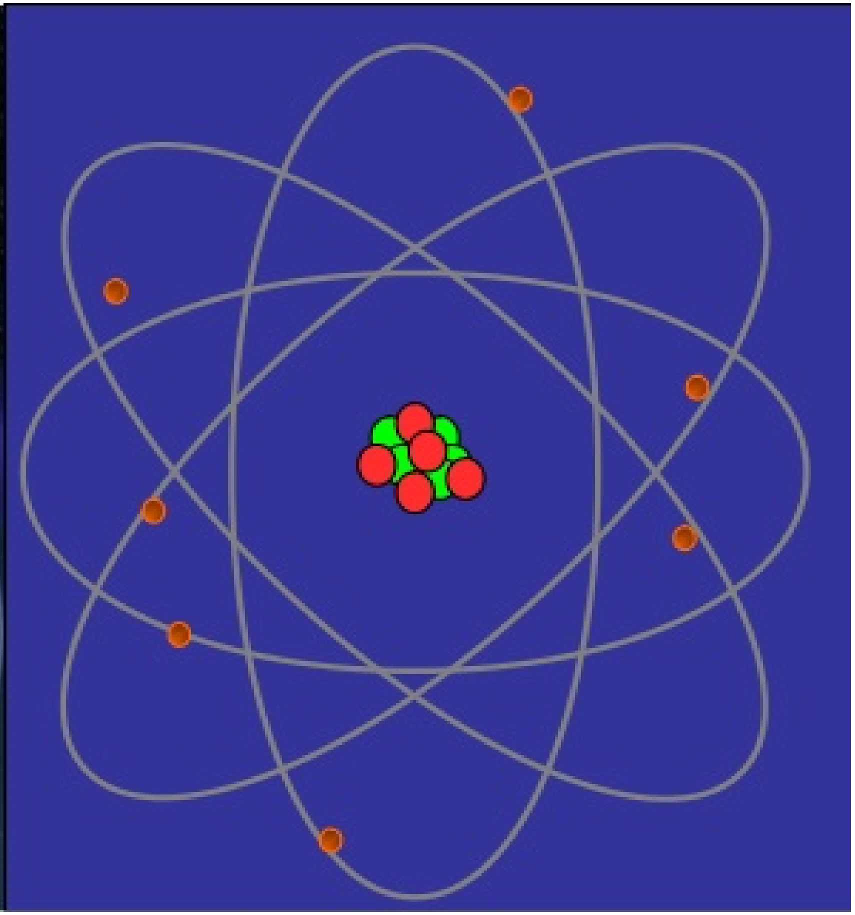


Planetary model of atom

Solar system

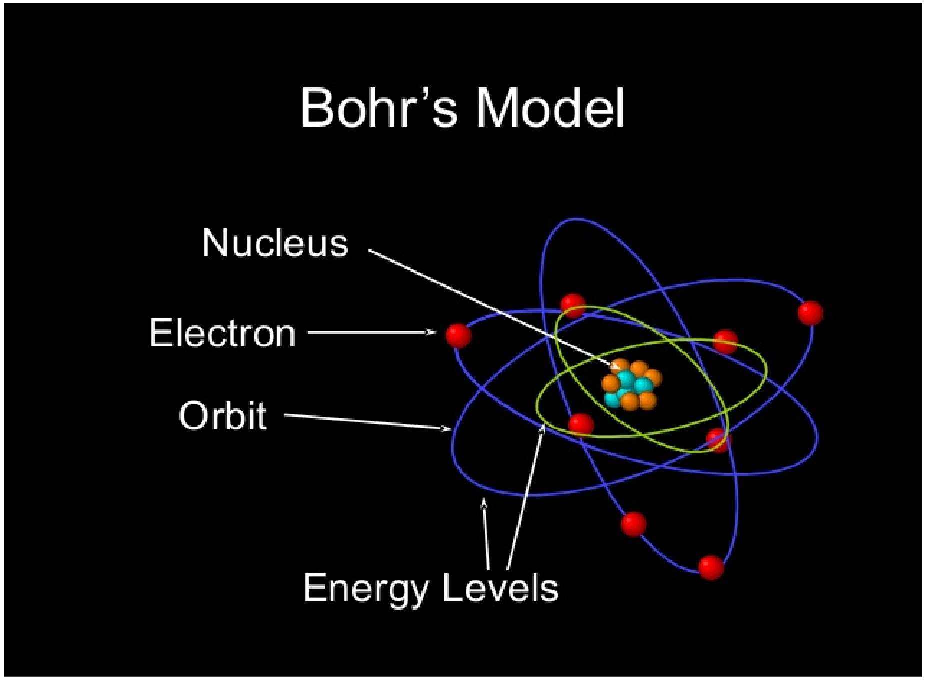


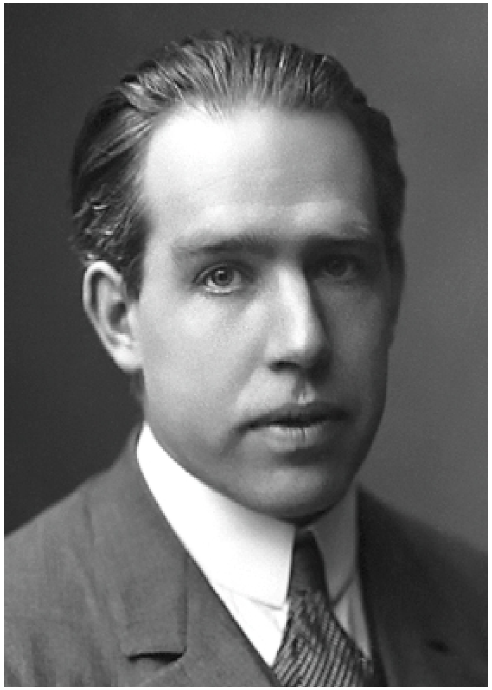
Rutherford's atom model



Bohr's model

- Electrons orbit the nucleus like planets orbit the sun
- Electrons fills the orbits closest to the nucleus
- Each orbit can hold a specific maximum number of electrons



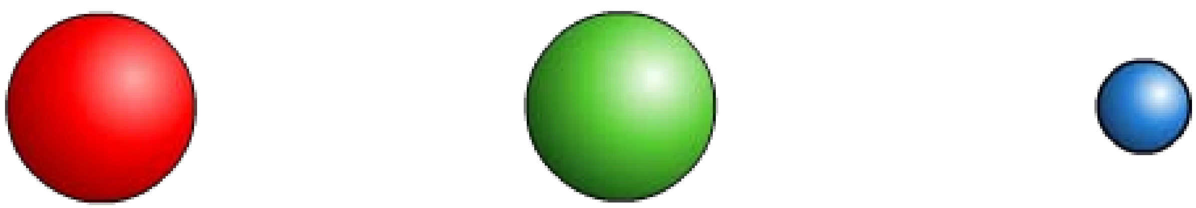


1885 –1962

What particles are atoms made of?

For some time, people thought that atoms were the smallest particles and could not be broken into anything smaller.

Scientists now know that atoms are actually made from even smaller particles. There are three types:



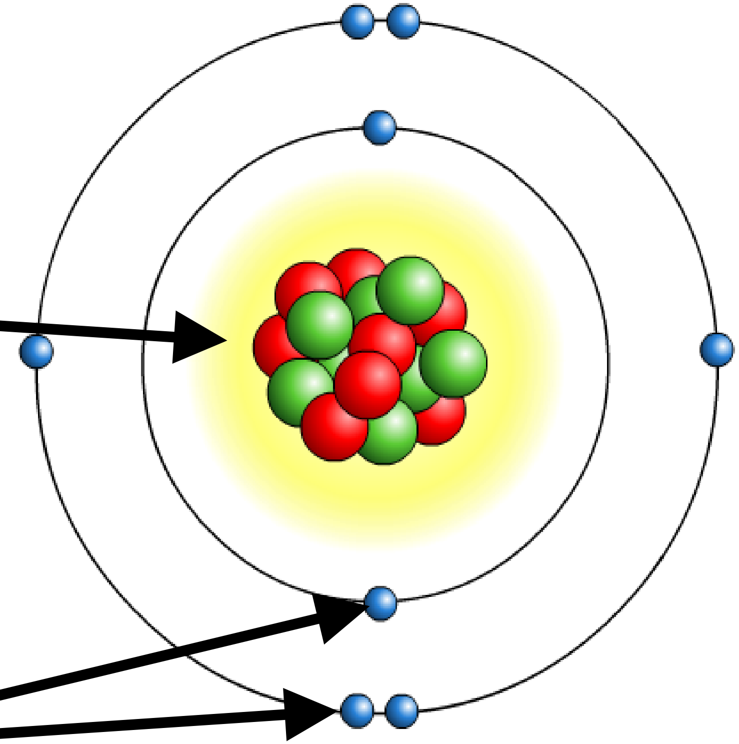
proton neutron electron

How are these particles arranged inside the atom?

What particles are atoms made of?

Protons, neutrons and electrons are not evenly distributed in an atom.

The protons and neutrons exist in a dense core at the centre of the atom. This is called the nucleus.



The electrons are spread out around the edge of the atom. They orbit the nucleus in layers called shells.

Every atom is composed of a nucleus and one or more electrons bound to the nucleus. The nucleus is made of one or more protons and typically a similar number of neutrons. Protons and neutrons are called nucleons. More than 99.94% of an atom's mass is in the nucleus. The protons have a positive electric charge, the electrons have a negative electric charge, and the neutrons have no electric charge. If the number of protons and electrons are equal, that atom is electrically neutral. If an atom has more or fewer electrons than protons, then it has an overall negative or positive charge, respectively, and it is called an ion.

These particles have the following properties:

Particle	Charge	Mass (g)	Mass (amu)
Proton	+1	1.6727×10^{-24} g	1.007316
Neutron	0	1.6750×10^{-24} g	1.008701
Electron	-1	9.110×10^{-28} g	0.000549

ATOMIC NUCLEOUS

The atomic nucleus is the positively electrified part of the atom. Regardless of its relatively small size, compared to the atom, it is concentrated almost the whole mass of the atom. The nucleus of the atoms consists of two types of particles - protons and neutrons, called total nucleons or nucleons.

Proton is a particle whose mass is approximately equal to the mass of a hydrogen atom. It has a positive charge that is denoted as (+1). The proton is indicated by the symbol **p** or **p⁺** .

The neutron is a material particle whose mass is also equal to the mass of the hydrogen atom (or proton). It does not carry an electric charge, it is electro neutral, and is denoted by the symbol **n** .

The number of protons is denoted as **Z** , And the number of neutrons with **N**. Therefore, the atomic mass A_M will be equal to the sum of the masses of the protons and the masses of neutrons that make up the nucleus, hence It is equal to the total mass of the nucleons

$$A_M = Z.m_{p+} + N.m_n$$

The sum $Z + N = A$, is called **mass number**.

ATOMIC NUCLEOUS

Z is an important individual feature of each chemical element. It is also called a sequential number or atomic number because it matches the sequence number of the element in the periodic system.

For example:

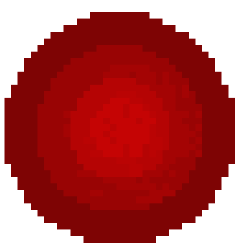
N (nitrogen)	has **7 p+**	and respectively	**Z = 7**
O (oxygen)	" **8 p+**	"	**Z = 8**
Na (sodium)	" **11 p+**	"	**Z = 11**

and so on.

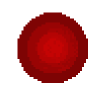
Generally (especially for lighter elements) **Z** = **N**, so if the sequence number of element **Z** and mass number ***A*** is known, the number of neutrons **N** can be determined. For heavier chemical elements the number of neutrons is greater than the number of protons.

Atomic Number (Z)

- This refers to how many protons an atom of that element has.
- No two elements, have the same number of protons.



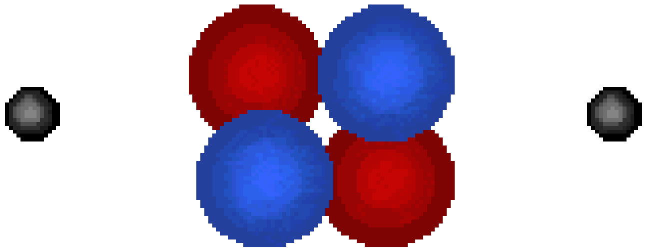
Bohr Model of Hydrogen Atom



Wave Model

Atomic Mass (A)

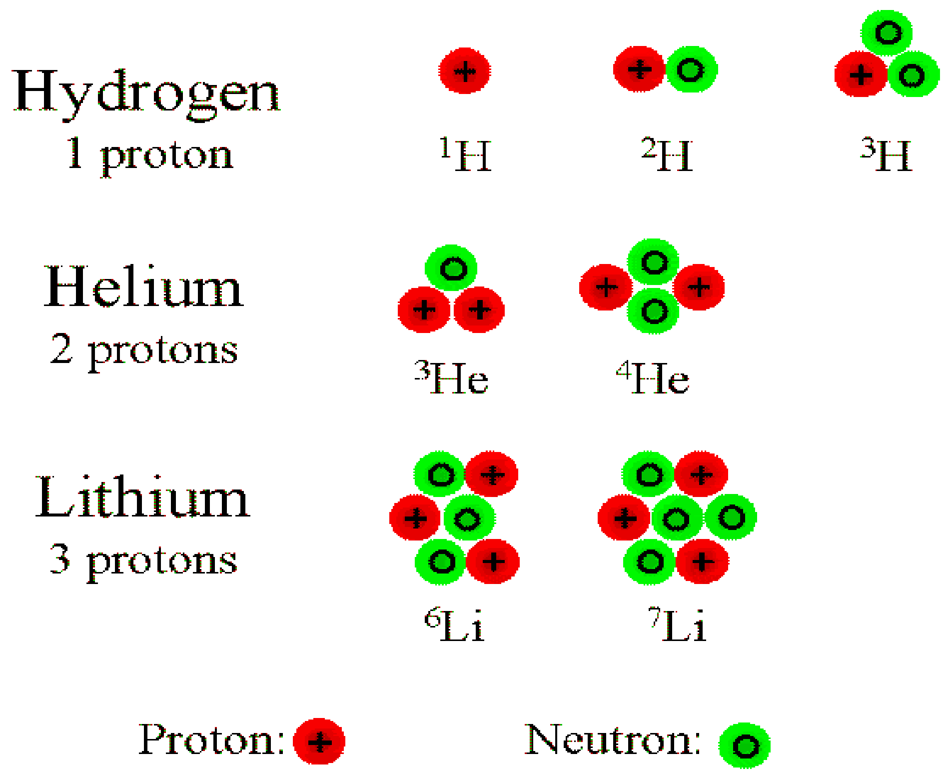
- Atomic Mass refers to the "weight" of the atom.
- It is derived at by adding the number of protons with the number of neutrons.



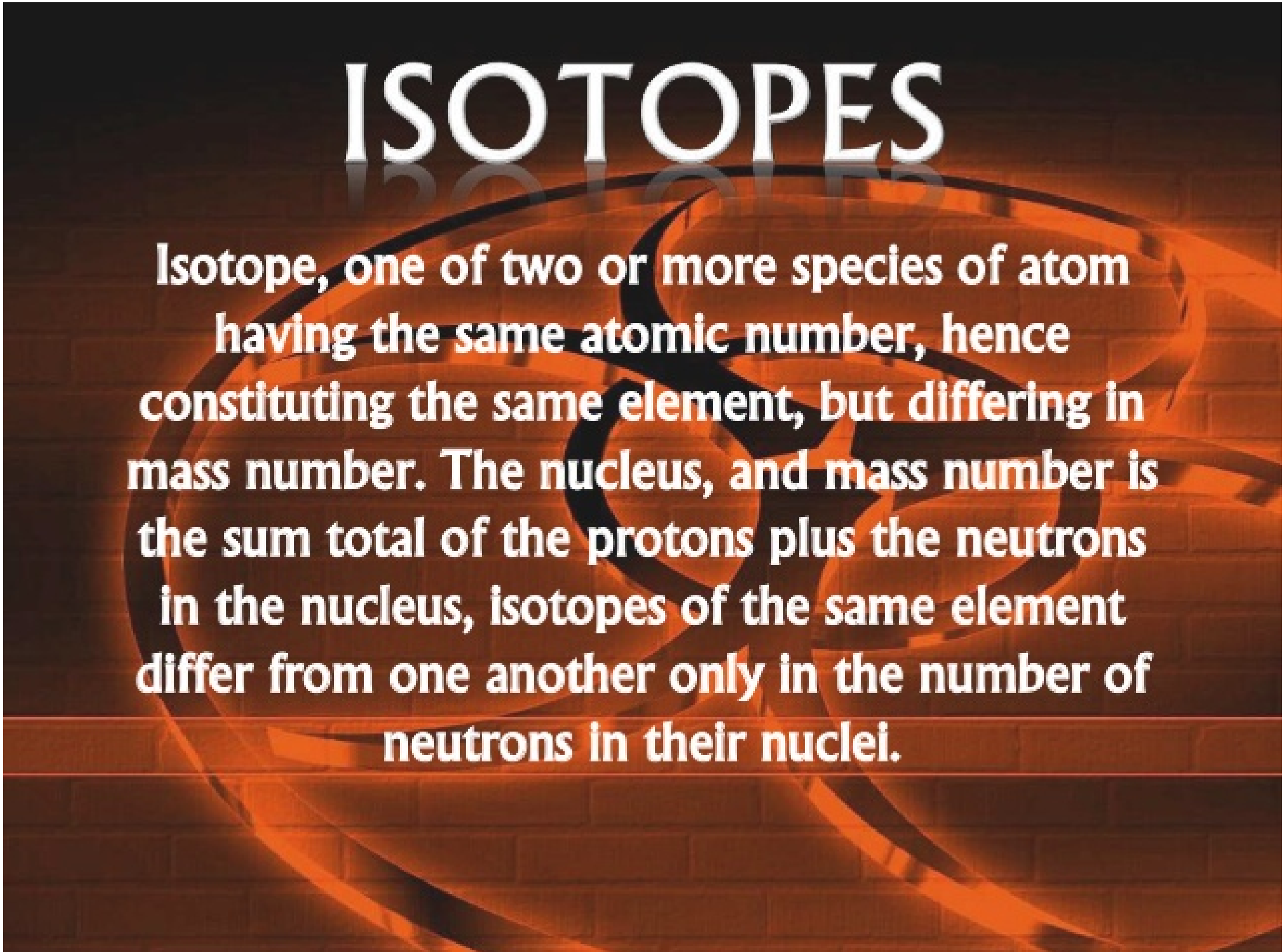
This is a helium atom. Its atomic mass is 4 (protons plus neutrons).

What is its atomic number?

Atomic Mass and Isotopes



- While most atoms have the same number of protons and neutrons, some don't.
- Some atoms have more or less neutrons than protons. These are called isotopes.
- An atomic mass number with a decimal is the total of the number of protons plus the *average* number of neutrons.


ISOTOPES
Isotope, one of two or more species of atom having the same atomic number, hence constituting the same element, but differing in mass number. The nucleus, and mass number is the sum total of the protons plus the neutrons in the nucleus, isotopes of the same element differ from one another only in the number of neutrons in their nuclei.

ISOBARS

The total number of nucleons is the same in the atoms of this pair of elements. Atoms of different elements with different atomic numbers, which have the same mass number, are known as isobars.

ATOMIC NUMBER (Z) = number of protons in nucleus

MASS NUMBER (A) = number of protons + number of neutrons

= atomic number (Z) + number of neutrons

ISOTOPS are atoms of the same element (X) with different numbers of neutrons in the nucleus

Mass Number $\rightarrow$ A

Atomic Number $\rightarrow$ Z

$^{A}_{Z}\mathrm{X}$ $\leftarrow$ Element Symbol

$^{1}_{1}\mathrm{H}$ $^{2}_{1}\mathrm{H}$ (D) $^{3}_{1}\mathrm{H}$ (T)

$^{235}_{92}\mathrm{U}$ $^{238}_{92}\mathrm{U}$

Atomic structure

- Atomic number
- Atomic mass

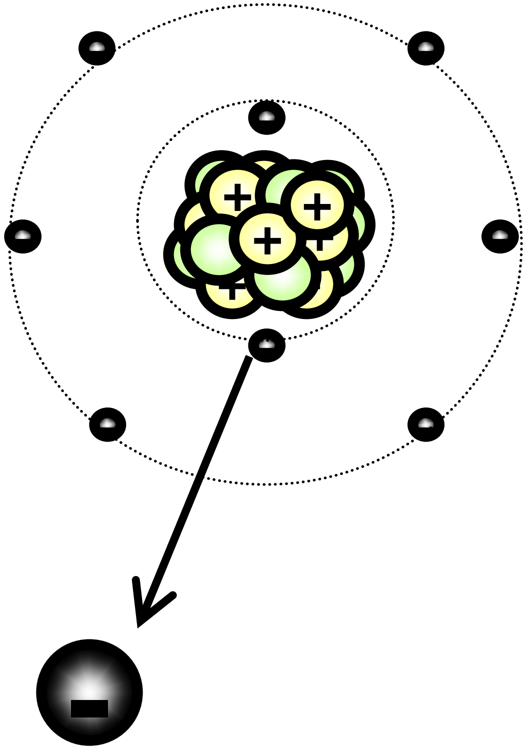
- Number of protons
- Number of protons + number of neutrons
- (isotopes vary in # neutrons)

- Number of electrons
- Electron energy levels
- # valence electrons

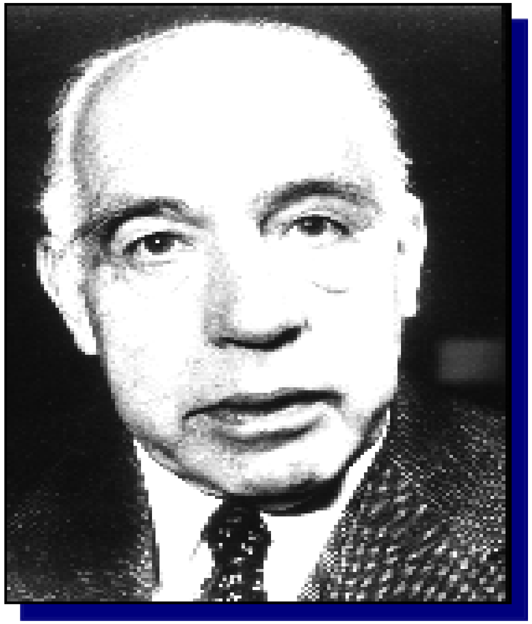
- Equal to # of protons
- Row on periodic table
- Group # (1-8)
- (active bonding electrons)

Electrons

- Negatively charged particles
- Found outside the nucleus of the atom, in the electron orbits/levels; each orbit/level can hold a maximum number of electrons (1^{st} = 2, 2^{nd} = 8, 3^{rd} = 8 or 18, etc…)
- Move so rapidly around the nucleus that they create an electron cloud
- Mass is insignificant when compared to protons and neutrons
- Equal to the number of protons
- Involved in the formation of chemical bonds



Atomic Line Spectra

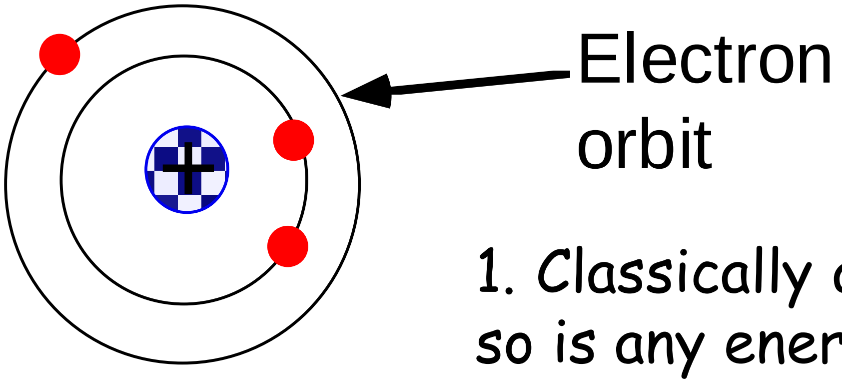


Niels Bohr (1885-1962)
(Nobel Prize, 1922)

- Bohr's greatest contribution to science was in building a simple model of the atom.
- It was based on understanding the SHARP LINE SPECTRA of excited atoms.
  - Excited atoms emit light of only certain wavelengths
  - The wavelengths of emitted light depend on the element.

Atomic Spectra and Bohr Model

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



1. Classically 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!

Atomic Spectra and Bohr Model

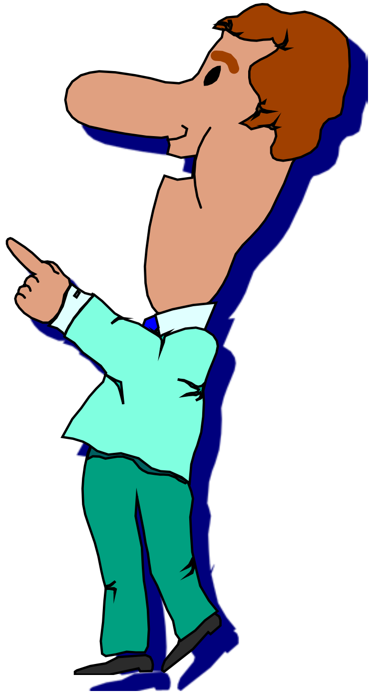
- Bohr said classical view is wrong.
- Need a new theory — now called QUANTUM or WAVE MECHANICS.
- e- can only exist in certain discrete orbits
  — called stationary states.
- e- is restricted to QUANTIZED energy states.

Energy of state = $- C/n^2$ where
  C is a CONSTANT
  n = QUANTUM NUMBER, n = 1, 2, 3, 4, ...

Atomic Spectra and Bohr Model

Energy of quantized state = $-C/n^2$

- Only orbits where n = integral number are permitted.
  - Radius of allowed orbitals
    = $n^2 \times (0.0529\ \text{nm})$
  - Results can be used to explain atomic spectra.



Quantum or Wave Mechanics

L. de Broglie
(1892-1987)

- Light has both wave & particle properties
- de Broglie (1924) proposed that all moving objects have wave properties.
- For light: E = hn = hc / l
- For particles: $E = mc^2$ (Einstein)

Therefore, $\boxed{mc = h / l}$

and for particles
$\boxed{\text{(mass)x(velocity)} = h / l}$

l for particles is called the de Broglie wavelength

I. Waves and Particles

- De Broglie's Hypothesis
  - Particles have wave characteristics
  - Waves have particle characteristics
  - ʎ = h/mn

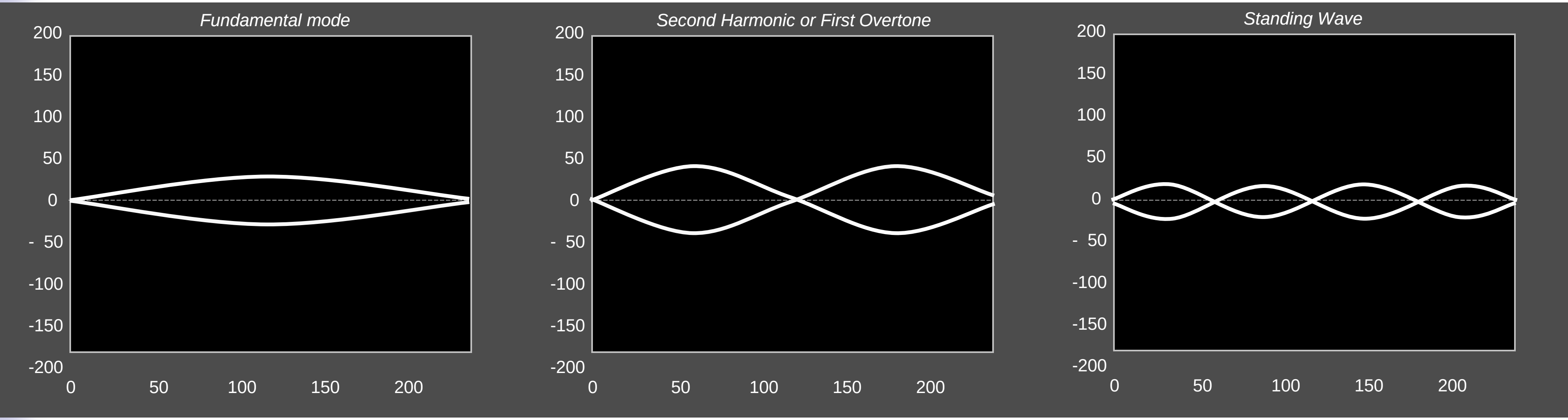
- Wave-Particle Duality of Nature
- Waves properties are significant at small momentum

Electrons as Waves

Louis de Broglie
~1924

- Louis de Broglie (1924)
  - Applied wave-particle theory to electrons
  - electrons exhibit *wave* properties

QUANTIZED WAVELENGTHS



Adapted from work by Christy Johannesson www.nisd.net/communicationsarts/pages/chem

From Bohr model to Quantum mechanics

Bohr's theory was a great accomplishment and radically changed our view of matter.

But problems existed with Bohr theory —

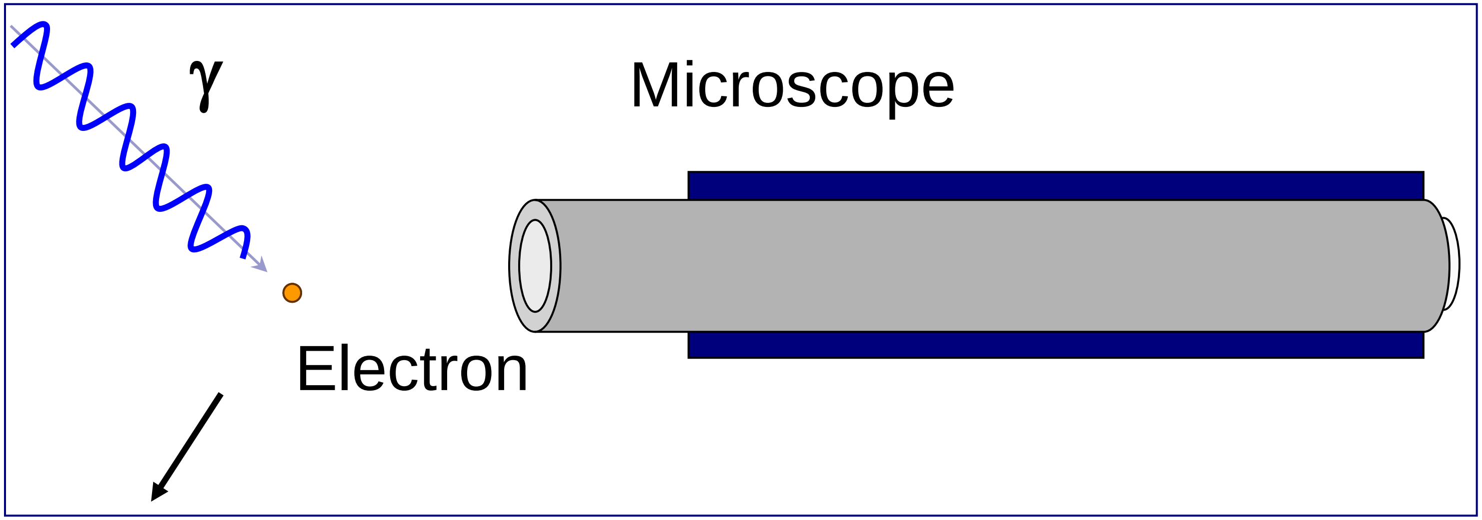
- theory only successful for the H atom.
- introduced quantum idea artificially.

- So, we go on to QUANTUM or WAVE MECHANICS

Quantum Mechanics

Werner Heisenberg
~1926

- Heisenberg Uncertainty Principle
  - Impossible to know both the *velocity* and *position* of an electron at the same time



$$(\Delta x)\,[\Delta(mv)] \geq \frac{h}{4\pi}$$

Uncertainty Principle

W. Heisenberg
1901-1976

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

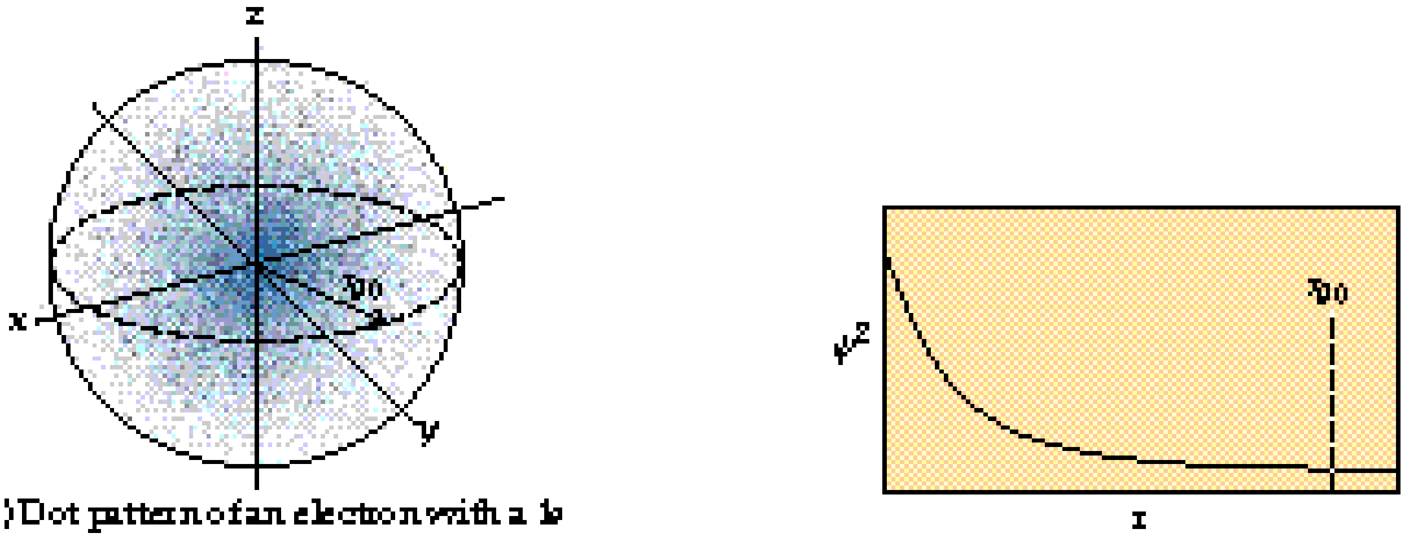
Cannot simultaneously define the position and momentum (= m•v) of an electron.

$$\Delta x.\ \Delta p = h$$

At best we can describe the position and velocity of an electron by a

PROBABILITY DISTRIBUTION, which is given by Ψ^2

Wavefunctions



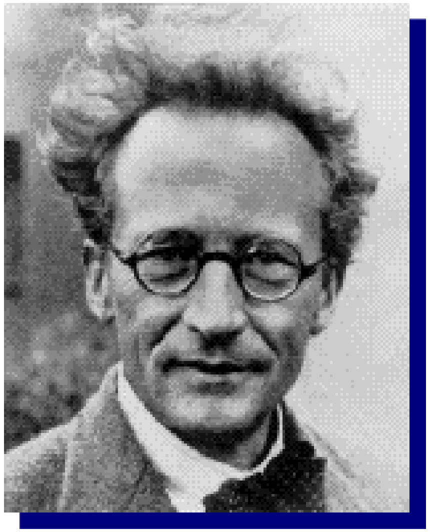
(a) Dot pattern of an electron with a 1s atomic orbital. Each dot represents the position of the electron at a different instant in time.

(b) A plot of the probability density as a function of distance for a one-electron atom with a 1s electron.

Ψ^2 is proportional to the probability of finding an e- at a given point.

Quantum or Wave Mechanics

II. The electron as a wave



E. Schrodinger
1887-1961

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

Solution to WAVE EQUATION gives set of mathematical expressions called

WAVE FUNCTIONS, Ψ

Each describes an allowed energy state of an e-

Quantization introduced naturally.

Quantum Mechanics

Erwin Schrödinger
~1926

- **Schrödinger Wave Equation** (1926)
  - finite # of solutions $\Rightarrow$ *quantized* energy levels
  - defines *probability* of finding an electron

$$\Psi_{1s} = \frac{1}{\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2} e^{-\sigma}$$

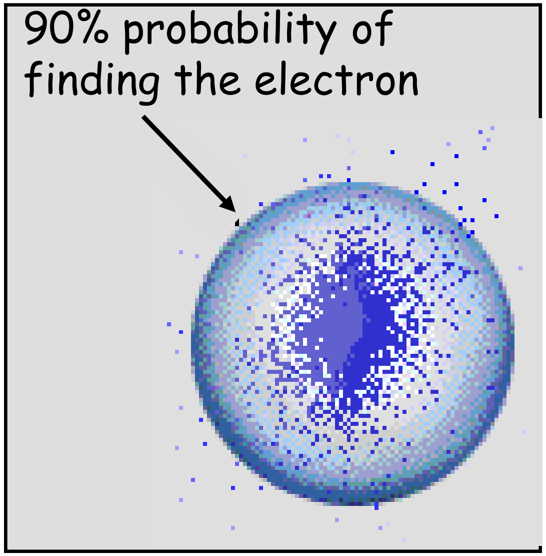
Courtesy Christy Johannesson www.nisd.net/communicationsarts/pages/chem

WAVE FUNCTIONS, Ψ

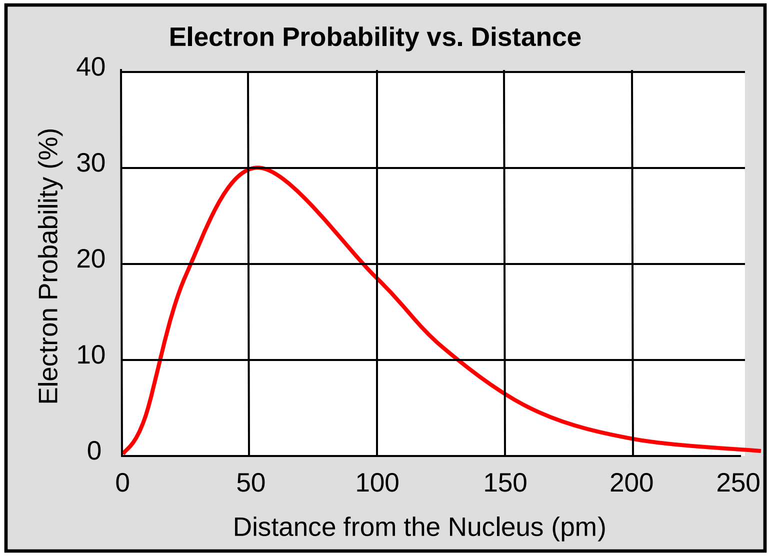
- Ψ is a function of distance and two angles.
- For 1 electron, Ψ corresponds to an ORBITAL — the region of space within which an electron is found.
- Ψ does NOT describe the exact location of the electron.
- Ψ^2 is proportional to the probability of finding an e- at a given point.

Quantum Mechanics

- **Orbital** ("electron cloud")
  - Region in space where there is 90% probability of finding an electron



Orbital



Courtesy Christy Johannesson www.nisd.net/communicationsarts/pages/chem

All the electrons are considered the same. In a multi-electron system, however, whatever the atom of each electron corresponds to a particular electron cloud. Therefore, each electron is characterized by its energy and an electronic cloud of certain shape, dimensions, spatial orientation, and distribution of the electronic density in it. These parameters determine the state of the electron in the electron shell of the atom.

The task of determining the state of the electrons in the electronic layer has been mathematically determined originally for the H atom using the Schrodinger equation. It turns out that this is a very difficult and not always solvable task. Moreover, the mathematical appearance of this equation is that it has countless solutions. However, only those that have a real physical meaning, consistent with the wave properties of the electron, must be selected.

As a result of these limitations, only certain energy values E and corresponding values for the wave function, i.e. For the distribution of electronic density. These solutions of the equation bear the name of their own values of E, respectively - their own wave function.

Orbital Quantum Numbers

Obtaining this set of own values that results from observing the boundary conditions of the wave function is associated with the input of three quantum numbers:

major - n, angular - l and magnetic - m .

Thus arranging the electrons in shells and subshells of ORBITALS, where

$n \rightarrow$ shell

$l \rightarrow$ subshell

$m_l \rightarrow$ designates an orbital within a subshell

Quantum Numbers

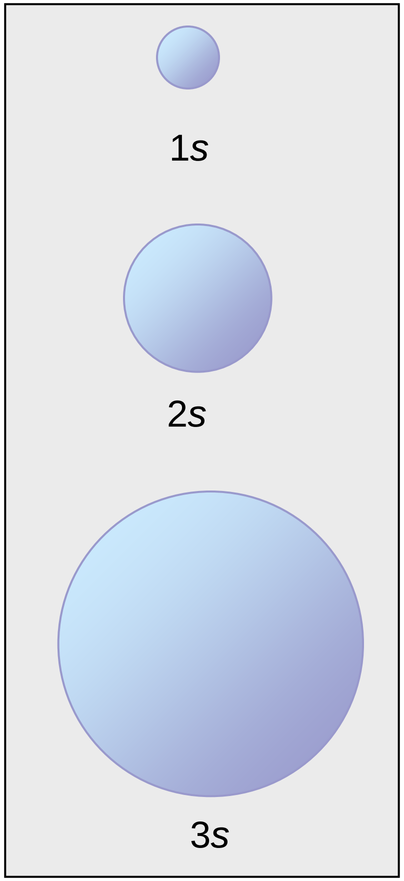
Symbol	Values	Description
n (major)	1, 2, 3, ..	Orbital size and energy = $-R(1/n^2)$
l (angular)	0, 1, 2, .. n-1	Orbital shape or type (subshell)
m_l (magnetic)	-l..0..+l	Orbital orientation in space

Total # of orbitals in l^{th} subshell = 2 l + 1

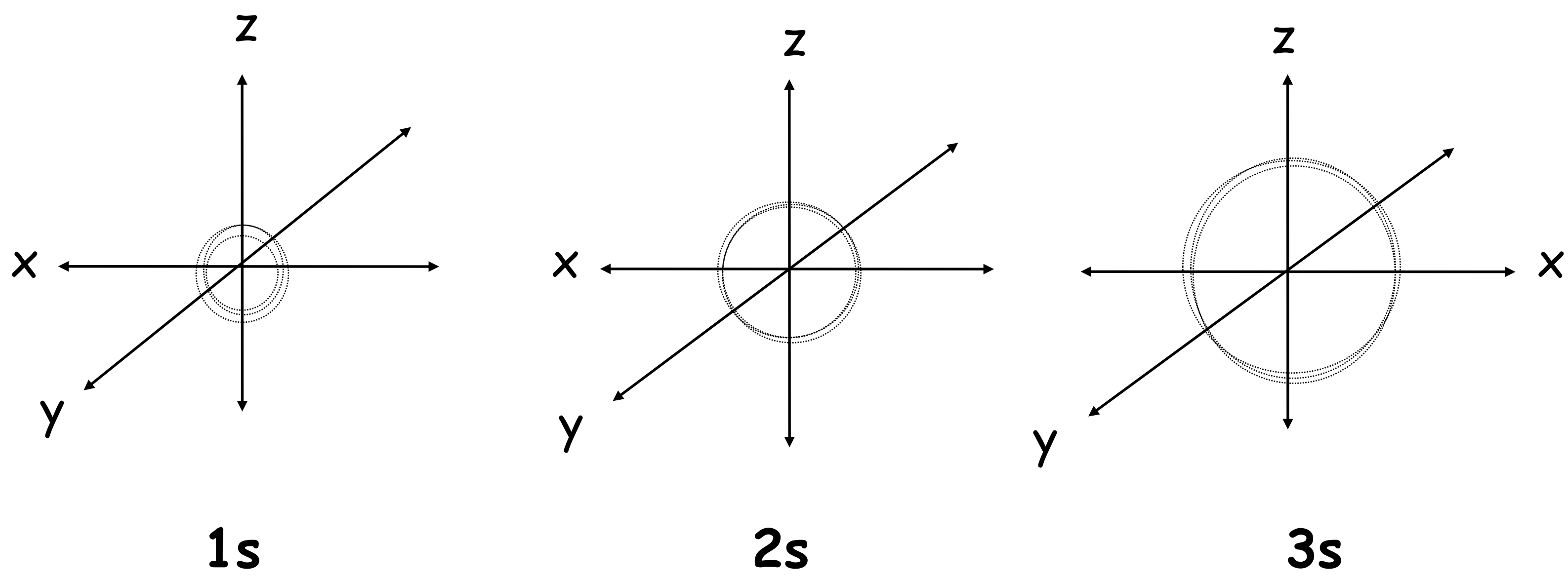
Quantum Numbers

1. Principal Quantum Number (*n*)

- Energy level
- Size of the orbital
- n^2 = # of orbitals in the energy level



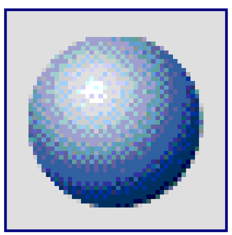
Major quantum number - n: Takes values of integers from 1, 2, 3 ... to ∞ . It is related to the **E** of the electron and the dimensions of the electronic cloud. The larger the **E**, the greater the **n**. In the same order, the dimensions of the electronic clouds also grow:



Quantum Numbers

2. Angular Momentum Quantum # (l)

- Energy sublevel
- Shape of the orbital



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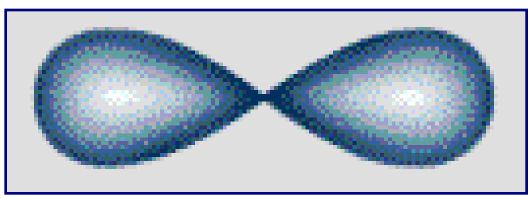

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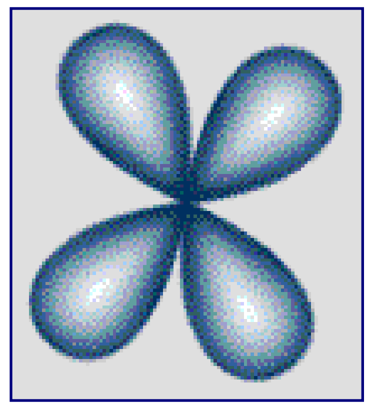

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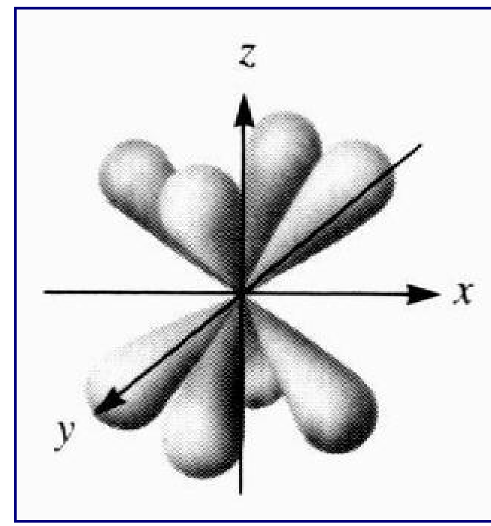


f

The azimuthal quantum number

Second quantum number *l is* called the **azimuthal quantum number**

- Value of *l* describes the *shape* of the region of space occupied by the electron

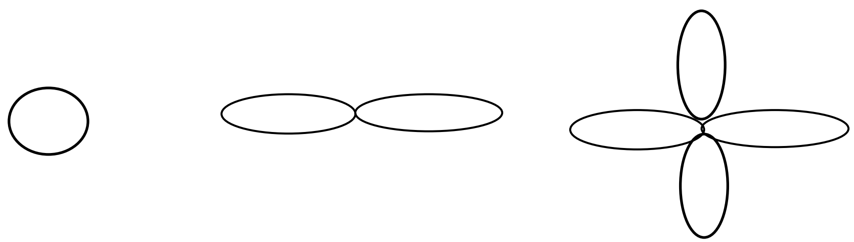
- Allowed values of *l* depend on the value of *n* and can range from 0 to *n* – 1

- All wave functions that have the same value of both *n* and *l* form a **subshell**

- Regions of space occupied by electrons in the same subshell have the same shape but are oriented differently in space

Angular quantum number - l: Takes values of integers from 0 to (n-1). With the exception of the H-atom, the orbital number l increases with an increase in the energy of the individual states. Above all, however, it takes into account the differences in the shape of electronic clouds. At l = 0, the electronic clouds are spherical and are called s-clouds; At l = 1 the shape is a spatial eight and the cloud is a p-shell; At l = 2 - respectively spatial four-leaf clover and respectively d-cloud; L = 3 - f - clouds with more complex shape, etc.

l =	**0**	**1**	**2**	**3**
designation	**s**	**p**	**d**	**f**

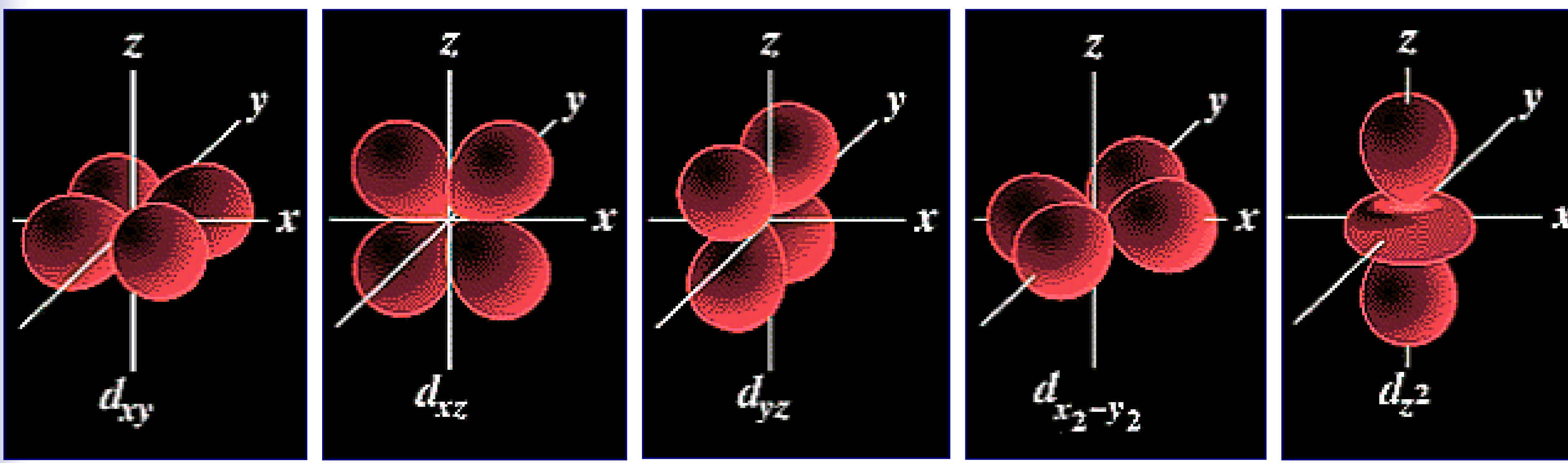


For example:

1s – defines		**n = 1**	**l = 0**	
2p	**"**	**n = 2**	**l = 1**	
4f	**"**	**n = 4**	**l = 3**	**etc.**

Quantum Numbers

3. Magnetic Quantum Number (m_l)
   - Orientation of orbital
   - Specifies the exact orbital within each sublevel

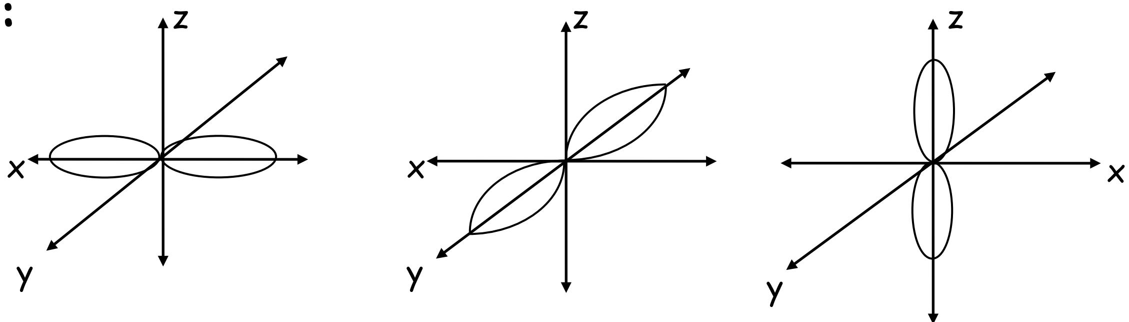


The magnetic quantum number

Third quantum is m_l, the **magnetic quantum number**

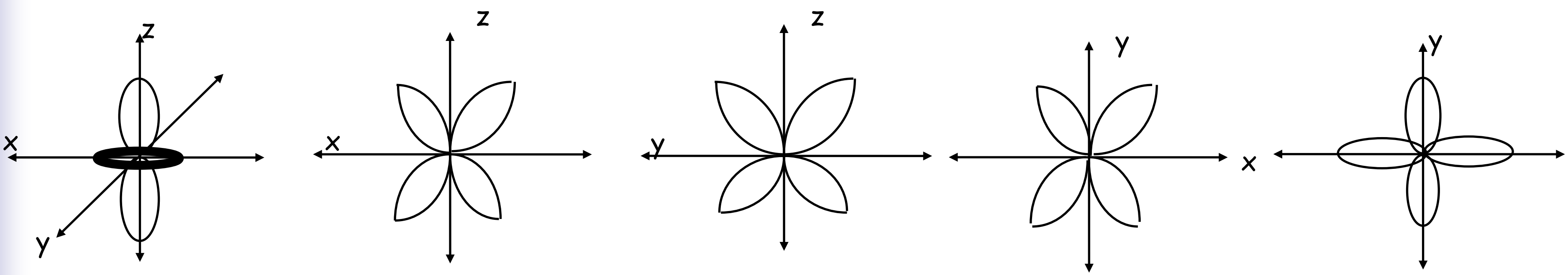
- Value of m_l describes the *orientation* of the region in space occupied by the electrons with respect to an applied magnetic field
- Allowed values of m_l depend on the value of l
- m_l can range from $-l$ to l in integral steps
  $m_l = -l, -l + 1, \ldots 0 \ldots, l - 1, l$
- Each wave function with an allowed combination of n, l, and m_l values describes an **atomic orbital**, a particular spatial distribution for an electron
- For a given set of quantum numbers, each principal shell contains a fixed number of subshells, and each subshell contains a fixed number of orbitals

Magnetic quantum number - m: adopts values of **l** (respectively of **n**) from **–l to +l**, including **0**, i.e. **(2l + 1)**-values. It is not related to the energy of the electron, but takes into account the shape and orientation of the electronic clouds in space. For example, the p-cloud can have three orientations in space, since the p-cloud value of **l = 1** and **m** having three values of **–1, 0, +1** respectively:



p_x(m = ± 1) p_y(m = ± 1) p_z(m = 0)

The same applies to d-electronic clouds corresponding to **l = 2** and **m = –2, –1, 0, +1, +2** , respectively. There are **5** orientations in space, and there is also a difference in shape:

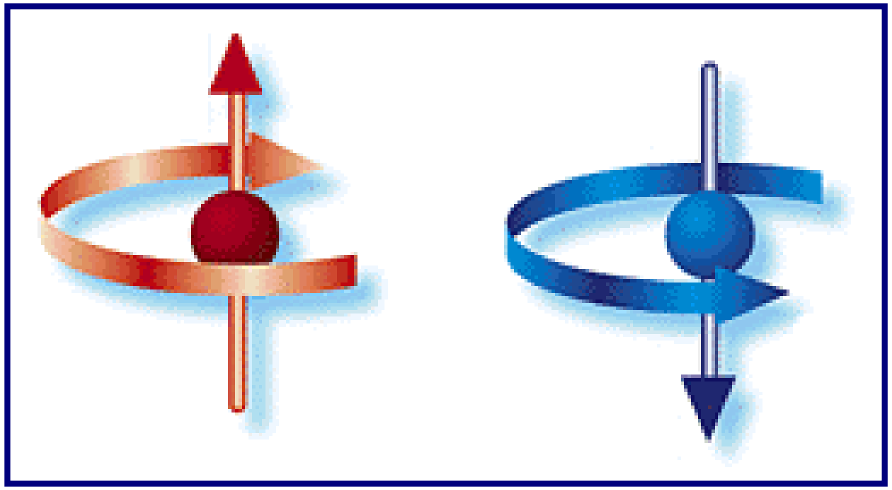


d_z (m=0) d_{xz}(m=±1) d_{yz}(m=±1) d_{xy}(m=±2) $d_{x2\ -\ y2}$ (m=±2)

Quantum Numbers

4. Spin Quantum Number (m_s)

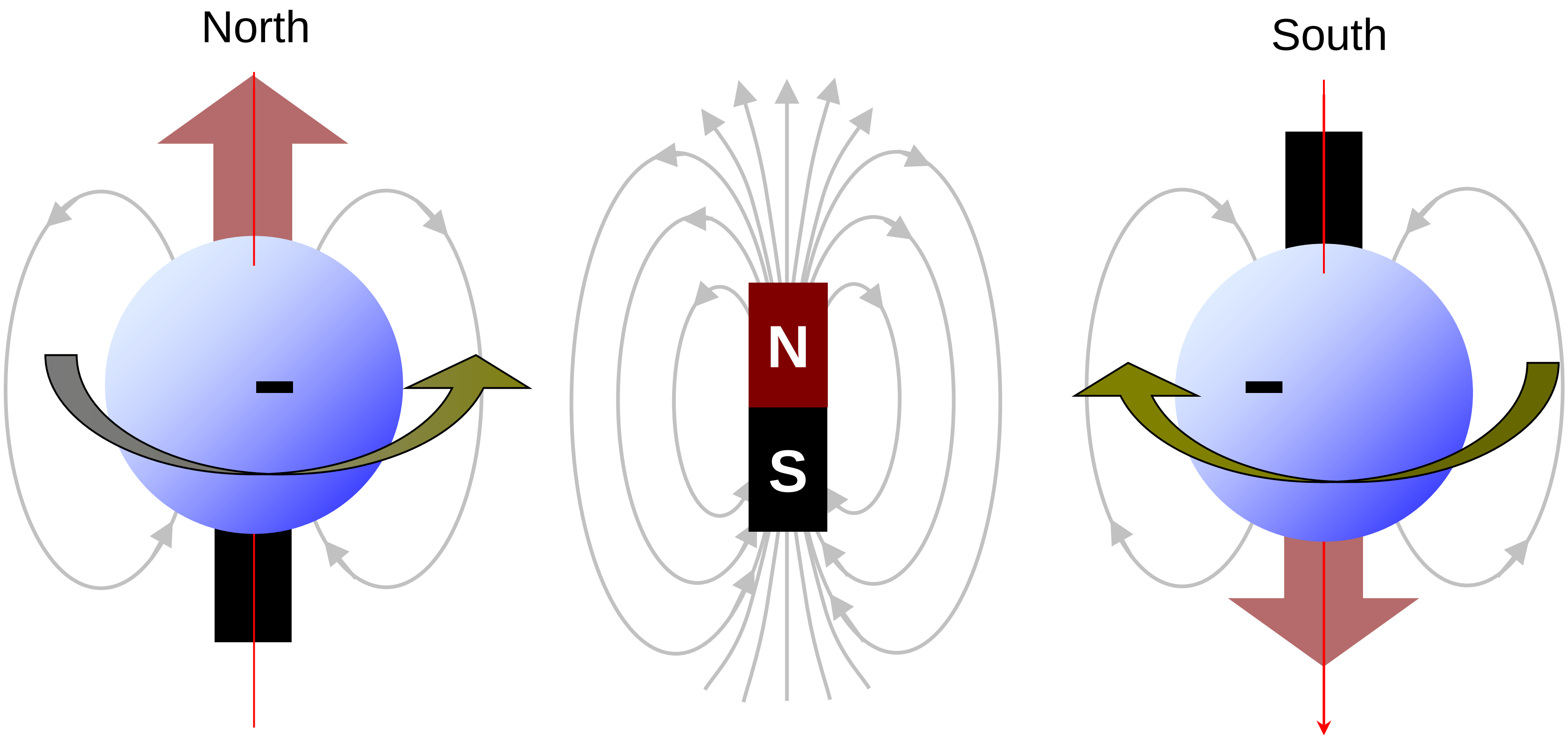
- Electron spin $\Rightarrow +\frac{1}{2}$ or $-\frac{1}{2}$
- An orbital can hold 2 electrons that spin in opposite directions.



Electron Spin: The Fourth Quantum Number

- When an electrically charged object spins, it produces a magnetic moment parallel to the axis of rotation and behaves like a magnet.
- A magnetic moment is called ***electron spin.***
- An electron has two possible orientations in an external magnetic field, which are described by a fourth quantum number $\boldsymbol{m_s}$.
- For any electron, m_s can have only two possible values, designated + (up) and – (down), indicating that the two orientations are opposite and the subscript *s* is for spin.
- An electron behaves like a magnet that has one of two possible orientations, aligned either with the magnetic field or against it.

Spin Quantum Number, m_s



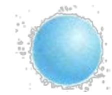
Electron aligned with magnetic field, $m_s = +\frac{1}{2}$

Electron aligned against magnetic field, $m_s = -\frac{1}{2}$

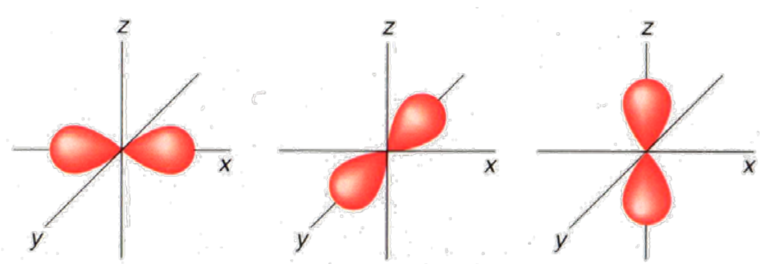
The electron behaves as if it were spinning about an axis through its center. This electron spin generates a magnetic field, the direction of which depends on the direction of the spin.

Shapes of s, p, and d-Orbitals

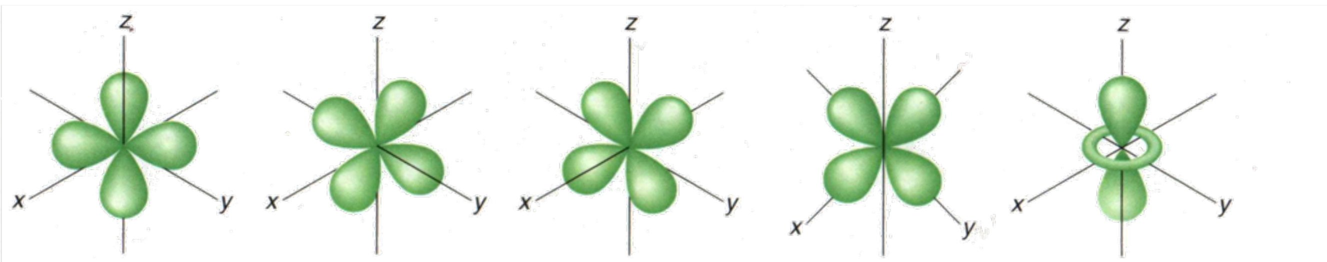
***s* orbital**



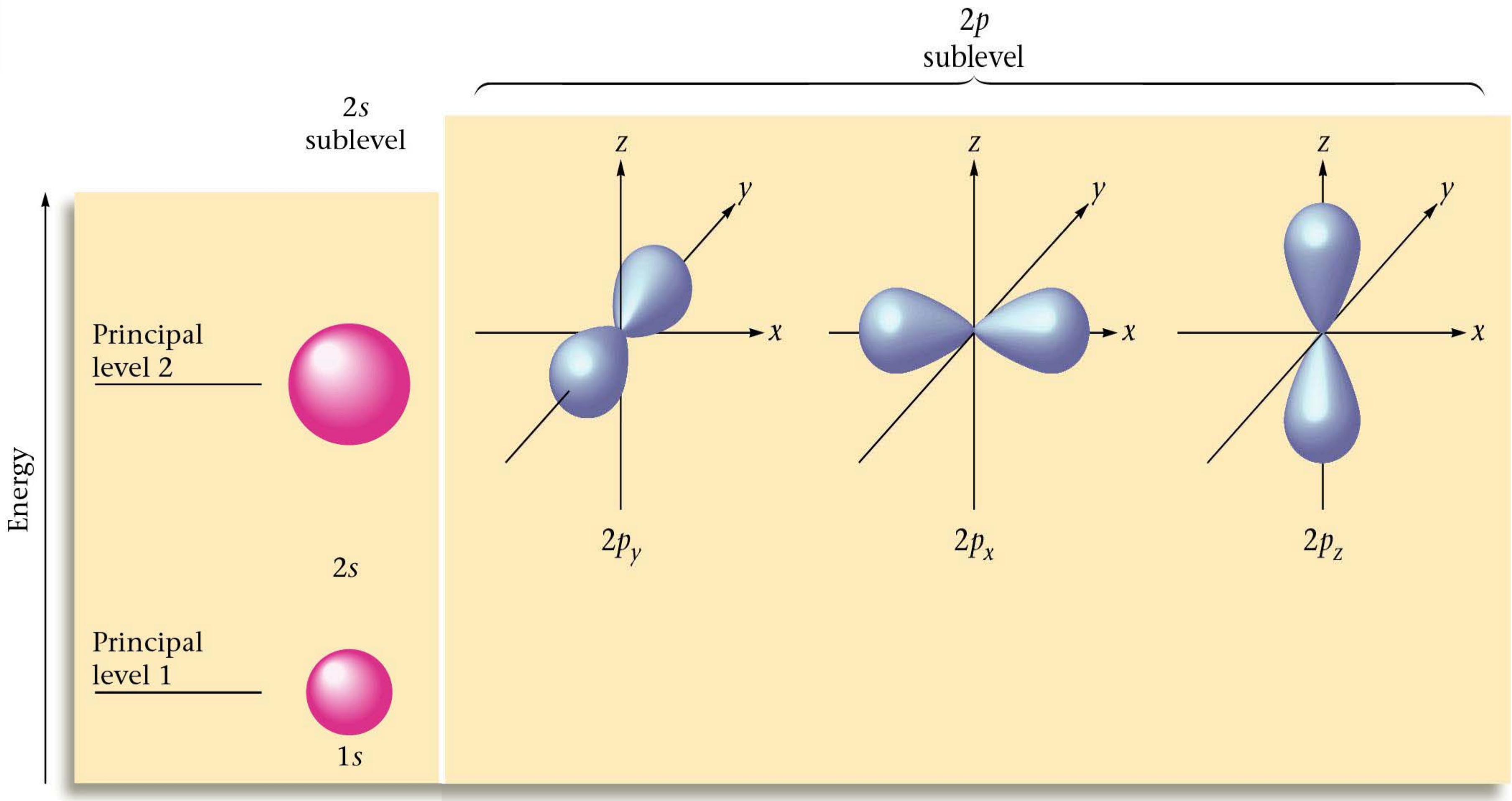
***p* orbitals**



***d* orbitals**



Principal Energy Levels 1 and 2



Filling Rules for Electron Orbitals

Aufbau Principle: Electrons are added one at a time to the lowest energy orbitals available until all the electrons of the atom have been accounted for.

Pauli Exclusion Principle: An orbital can hold a maximum of two electrons. To occupy the same orbital, two electrons must spin in opposite directions.

Hund's Rule: Electrons occupy equal-energy orbitals so that a maximum number of unpaired electrons results.

**Aufbau* is German for "building up"

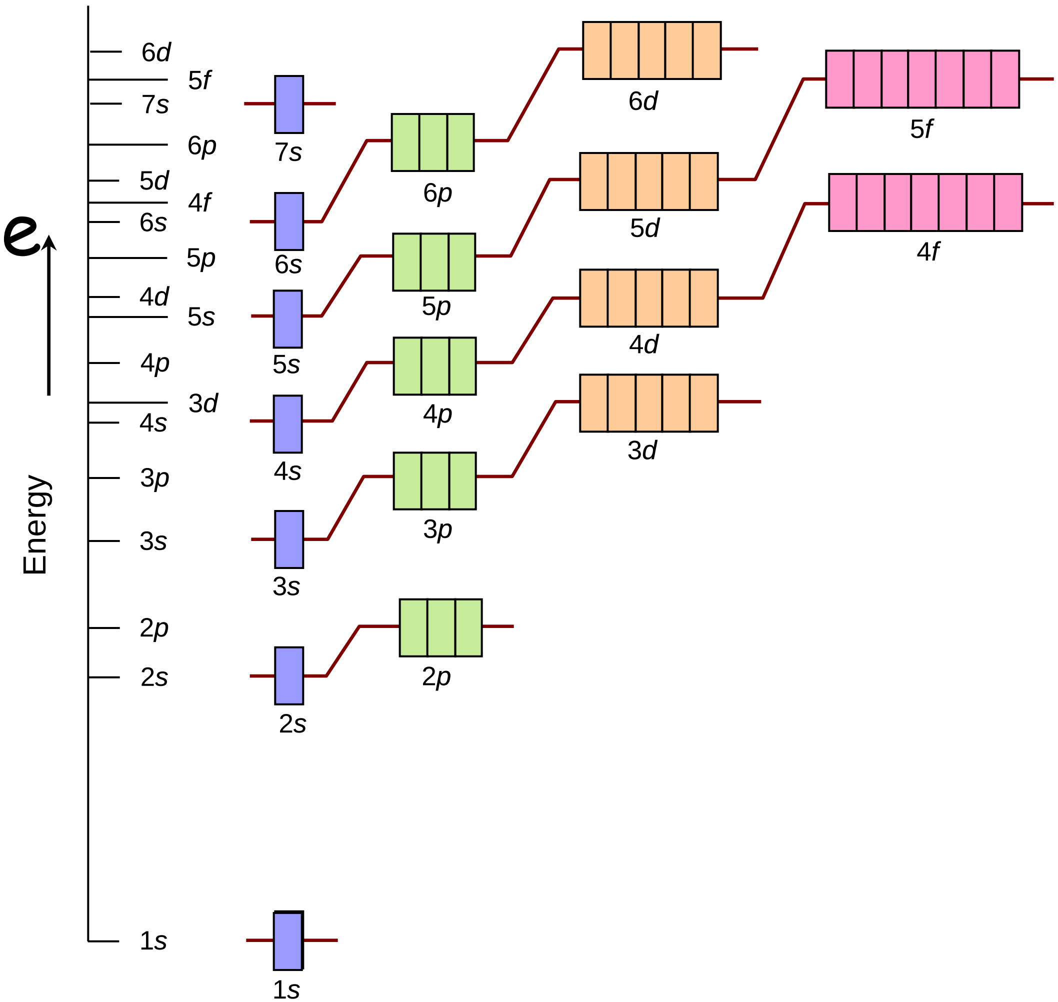
Maximum Number of Electrons In Each Sublevel

Sublevel	Number of Orbitals	Maximum Number of Electrons
s	1	2
p	3	6
d	5	10
f	7	14

General Rules

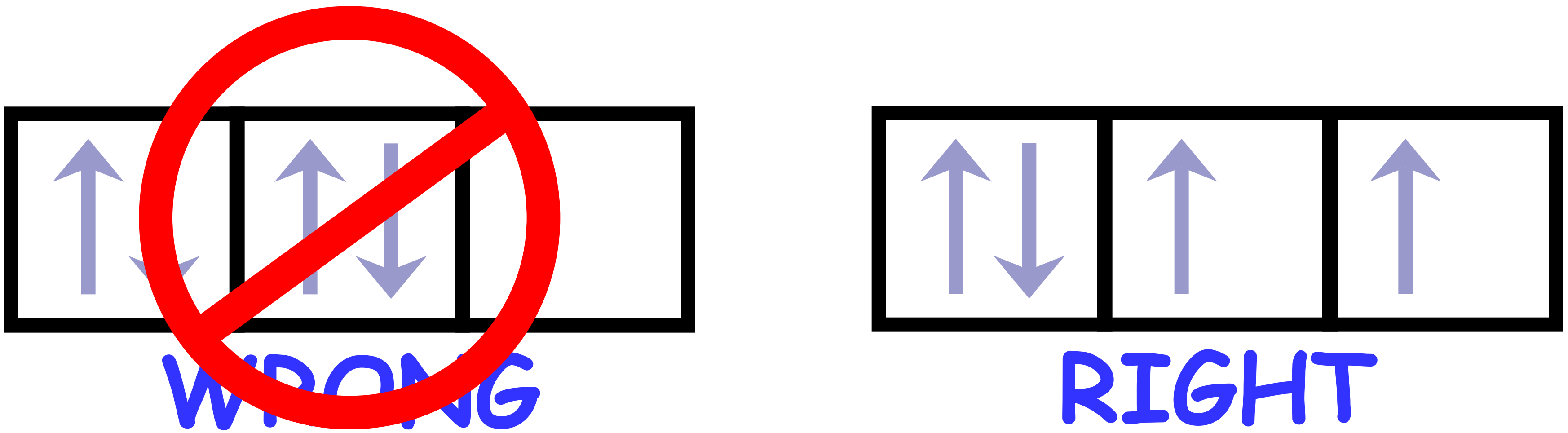
Aufbau Principle

- Electrons fill the lowest energy orbitals first.
- "Lazy Tenant Rule"



General Rules

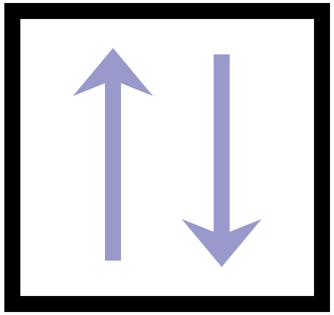
- Hund's Rule
  - Within a sublevel, place one electron per orbital before pairing them.
  - "Empty Bus Seat Rule"



General Rules

Wolfgang Pauli

- Pauli Exclusion Principle
  - Each orbital can hold TWO electrons with opposite spins.



Writing Atomic Electron Configurations

Two ways of writing configs.

One is called the spdf notation.

spdf notation

for H, atomic number = 1

$1s^1$

no. of electrons

value of n

value of l

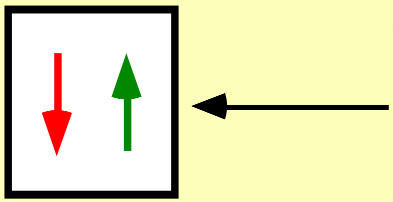
Writing Atomic Electron Configurations

Two ways of writing configs.

Other is called the orbital box notation.

ORBITAL BOX NOTATION
for He, atomic number = 2

$1s^2$



1s

Arrows depict electron spin

One electron has $n = 1$, $l = 0$, $m_l = 0$, $m_s = + 1/2$

Other electron has $n = 1$, $l = 0$, $m_l = 0$, $m_s = - 1/2$