

CHAPTER-6 Structure of Atom

Bohr's model of hydrogen atom

Main Postulates:

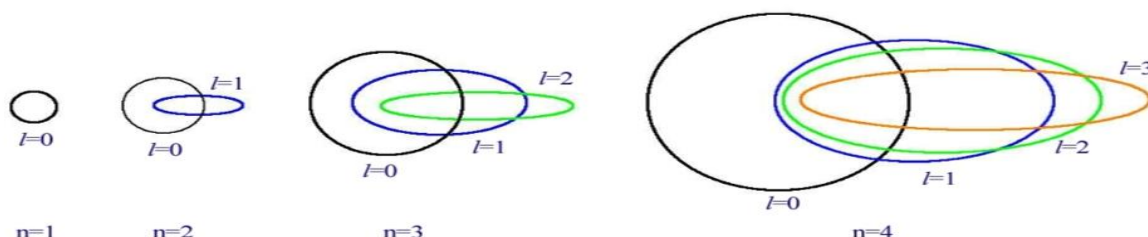
1. Niels Bohr proposed that electrons in an atom occupy 'stationary orbitals(states) of fixed energy at different distances from the nucleus.
2. When an electron jumps from a lower energy(ground state) to higher energy states(excited state) it absorbs energy or emits energy when such a jump occurs from a higher energy state to a lower energy state.
3. The energies of an electron in an atom can have only certain values E_1, E_2, E_3, \dots ; that is, the energy is quantized. The states corresponding to these energies are called stationary states and the possible values of the energy are called energy levels.

Limitations:

1. Bohr's model failed to account for splitting of line spectra of hydrogen atom into finer lines.
2. Bohr's model could not explain the Zeeman and stark effects.

Bohr-Sommerfeld model of an atom

1. In an attempt to account for the structure (splitting) of line spectra known as fine spectra, Sommerfeld modified Bohr's atomic model by adding elliptical orbits.
2. While retaining the first of Bohr's circular orbit as such, he added one elliptical orbit to Bohr's second orbit, two elliptical orbits to Bohr's third orbit, etc., such that the nucleus of the atom is one of the principal foci of these elliptical orbits.
3. He was guided by the fact that, in general, periodic motion under the influence of a central force will lead to elliptical orbits with the force situated at one of the foci.



Limitations:

1. This model failed to account for the atomic spectra of atoms of more than one electron.

Quantum numbers

Each electron in an atom is described by a set of three numbers $n, l,$ and m_l . These numbers are called quantum numbers. The quantum numbers describe the space around the nucleus where the electrons are found and also their energies. These are called atomic orbitals.

1. Principal Quantum Number (n)

- The principal quantum number is related to the size and energy of the main shell and it is denoted by n .
- ' n ' has positive integer values of 1, 2, 3,...
- As ' n ' increases, the shells become larger and the electrons in those shells are farther from the nucleus.
- An increase in ' n ' also means higher energy. $n = 1, 2, 3, \dots$ are often represented by the letters K, L, M... For each ' n ' value there is one main shell.

Shell	K	L	M	N
n	1	2	3	4

2. The angular - momentum quantum number (l)

- The angular momentum quantum number ' l ' has integer values from 0 to $n-1$ for each value of ' n '.
- Each ' l ' value represents one sub-shell.
- Each value of ' l ' is related to the shape of a particular sub-shell in the space around the nucleus.
- The value of ' l ' for a particular sub-shell is generally designated by the letters s, p, d . . . as follows: 1 0 1 2 3
- When $n = 1$, there is only one sub-shell with $l = 0$. This is designated as '1s' orbital.
- When $n = 2$, there are two sub-shells, with $l = 0$, the '2s' sub-shell and with $l = 1$, the '2p' sub-shell.

l	0	1	2	3
Name of the sub-shell	s	p	d	f

3. The magnetic quantum number (m_l)

- The magnetic quantum number (m_l) has integer values between -1 and 1, including zero. Thus for a certain value of l , there are $(2l + 1)$ integer values of m_l as follows:
-1, (-1+1) . . . , -1, 0, 1, . . . (+1 - 1), +1
- These values describe the orientation of the orbital in space relative to the other orbitals in the atom.
- When $l = 0$, $(2l + 1) = 1$ and there is only one value of m_l , thus we have only one orbital i.e., 1s.
- When $l = 1$, $(2l + 1) = 3$, that means m_l has three values, namely, -1, 0, and 1 or three p orbitals, with different orientations along x, y, z axes. These are labelled as p_x , p_y , and p_z .
- The number of ' m_l ' values indicates the number of orbitals in a sub-shell with a particular l value. Orbitals in the sub-shell belonging to the same shell possess same energy. These are called degenerated orbitals.
- s-orbital is spherical in shape, p-orbital is dumbbell-shaped and d-orbital are double dumbbell-shaped

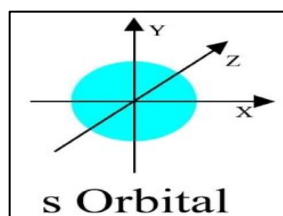
Sub shells	Number of orbitals ($2l+1$)	Maximum number of electrons
s ($l=0$)	1	2
p ($l=1$)	3	6
d ($l=2$)	5	10
f ($l=3$)	7	14

4. Spin Quantum Number (m_s)

- The three quantum numbers n , l , and m_l describe the size (energy), shape, and orientation, respectively, of an atomic orbital in space.
- This represents the property of the electron. It is denoted by ' m_s '.
- This quantum number refers to the two possible orientations of the spin of an electron, one clockwise and the other anticlockwise spin.
- These are represented by $+1/2$ and $-1/2$. If both are positive values, then the spins are parallel otherwise the spins are anti-parallel.

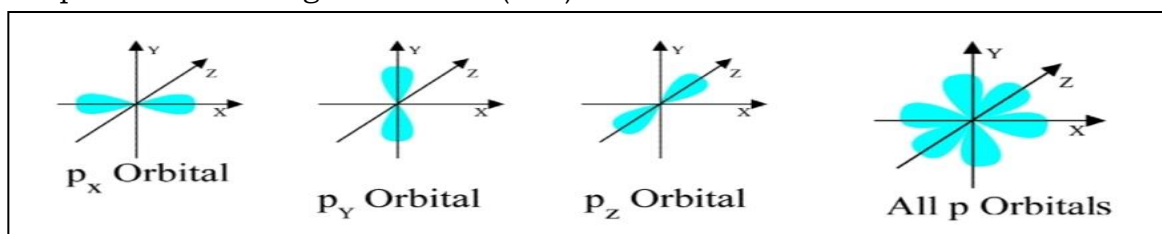
s-orbital

- s-orbital is spherical in shape
- $l=0$ represents s-orbital
- s-orbital starting from K-shell($n=1$)



p-orbitals

- p-orbital is dumbbell-shaped
- $l=1$ represents p-orbitals
- p-orbitals starting from L-shell($n=2$)



Electronic Configuration

The distribution of electrons in shells, sub-shells and orbitals in an atom is called the electronic configuration

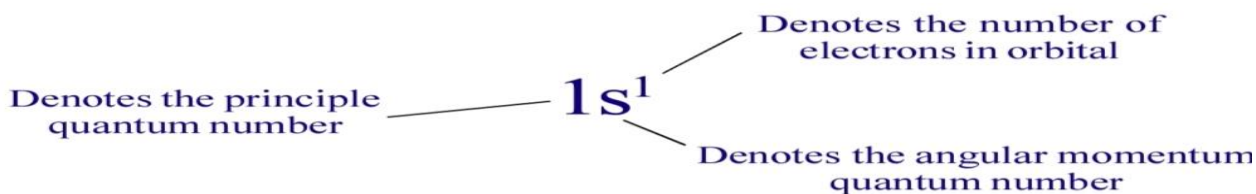
The electronic configuration of an atom gives

- The distribution of electrons in various atomic orbitals provides an understanding of the electronic behavior of the atom and, in turn, its reactivity.
- The electron configuration can also be represented by showing the spin of the electron.

$n l^x$ method

The shorthand notation consists of the principal energy level (n value), the letter representing sub-level (l value), and the number of electrons (x) in the sub-shell is written as a superscript as shown $n l^x$.

- For the hydrogen (H) atom having atomic number (Z) = 1, the number of electrons is one, then the electronic configuration is $1s^1$.



For the electron in H, as you have seen, the set of quantum numbers is $n = 1, l = 0, m_l = 0, m_s = \frac{1}{2}$ or $-\frac{1}{2}$.

Useful of $n l^x$ method:

1. To write the electronic configuration of an atom.
2. To find the position of electrons around the nucleus in an atom.

Pauli Exclusion Principle: According to Pauli Exclusion Principle no two electrons of the same atom can have all four quantum numbers the same.

Ex: The electronic configuration of Helium($Z=2$) is $1s^2$



Electron	n	l	m_l	m_s
1 st	1	0	0	+1/2
2 nd	1	0	0	-1/2

We observe that three quantum numbers are equal but fourth one is different

Aufbau Principle(Building up principle): The lowest-energy orbitals are filled first.

Two general rules help us to predict electronic configurations.

1. Electrons are assigned to orbitals in order of increasing value of $(n+l)$.
2. For sub-shells with the same value of $(n+l)$, electrons are assigned first to the sub-shell with lower 'n'.

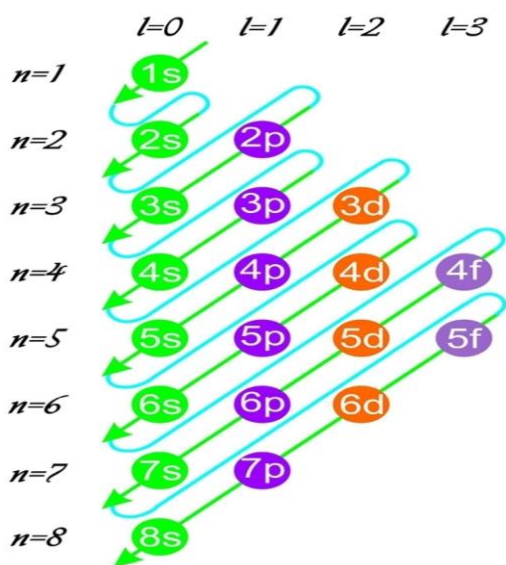
Ex: In Scandium($Z=21$), first twenty electrons can be accommodated in $1s, 2s, 2p, 3s, 3p$ and $4s$ orbitals. The last electron can enter into either $3d$ or $4p$ orbital

Orbital	$(n+l)$ value
3d	$3+2=5$
4p	$4+1=5$

Both orbitals have $(n+l)$ value. But $3d$ orbital is least "n" value. So last electron enter into $3d$ orbital.

Moeller Chart (The filling order of atomic orbitals): The following diagram shows the increasing value of $(n+l)$. Ascending order of energies of various atomic orbitals is given below.

$1s < 2s < 2p < 3s < 3p < 4s < 3d < 4p < 5s < 4d < 5p < 6s < 4f < 5d < 6p < 7s < 5f < 6d < 7p < 8s \dots$



Hund's Rule: According to this rule electron pairing in orbitals starts only when all available empty orbitals of the same energy (degenerate orbitals) are singly occupied.

1. The configuration of Carbon (C) atom ($Z=6$) is $1s^2 2s^2 2p^2$.
2. The first four electrons go into the $1s$ and $2s$ orbitals.
3. The next two electrons go into separate $2p$ orbitals, with both electrons having the same spin



Electronic configuration of First 30 elements

Element	Symbol	Atomic number(Z)	Electronic configuration
Hydrogen	H	1	1s ¹
Helium	He	2	1s ²
Lithium	Li	3	1s ² 2s ¹ (OR) [He]2s ¹
Beryllium	Be	4	1s ² 2s ² (OR) [He]2s ²
Boron	B	5	1s ² 2s ² 2p ¹ (OR) [He]2s ² 2p ¹
Carbon	C	6	1s ² 2s ² 2p ² (OR) [He]2s ² 2p ²
Nitrogen	N	7	1s ² 2s ² 2p ³ (OR) [He]2s ² 2p ³
Oxygen	O	8	1s ² 2s ² 2p ⁴ (OR) [He]2s ² 2p ⁴
Fluorine	F	9	1s ² 2s ² 2p ⁵ (OR) [He]2s ² 2p ⁵
Neon	Ne	10	1s ² 2s ² 2p ⁶
Sodium	Na	11	1s ² 2s ² 2p ⁶ 3s ¹ (OR) [Ne]3s ¹
Magnesium	Mg	12	1s ² 2s ² 2p ⁶ 3s ² (OR) [Ne]3s ²
Aluminium	Al	13	1s ² 2s ² 2p ⁶ 3s ² 3p ¹ (OR) [Ne]3s ² 3p ¹
Silicon	Si	14	1s ² 2s ² 2p ⁶ 3s ² 3p ² (OR) [Ne]3s ² 3p ²
Phosphorus	P	15	1s ² 2s ² 2p ⁶ 3s ² 3p ³ (OR) [Ne]3s ² 3p ³
Sulphur	S	16	1s ² 2s ² 2p ⁶ 3s ² 3p ⁴ (OR) [Ne]3s ² 3p ⁴
Chlorine	Cl	17	1s ² 2s ² 2p ⁶ 3s ² 3p ⁵ (OR) [Ne]3s ² 3p ⁵
Argon	Ar	18	1s ² 2s ² 2p ⁶ 3s ² 3p ⁶
Potassium	K	19	1s ² 2s ² 2p ⁶ 3s ² 3p ⁶ 4s ¹ (OR) [Ar]4s ¹
Calcium	Ca	20	1s ² 2s ² 2p ⁶ 3s ² 3p ⁶ 4s ² (OR) [Ar]4s ²
Scandium	Sc	21	1s ² 2s ² 2p ⁶ 3s ² 3p ⁶ 4s ² 3d ¹ (OR) [Ar]4s ² 3d ¹
Titanium	Ti	22	1s ² 2s ² 2p ⁶ 3s ² 3p ⁶ 4s ² 3d ² (OR) [Ar]4s ² 3d ²
Vanadium	V	23	1s ² 2s ² 2p ⁶ 3s ² 3p ⁶ 4s ² 3d ³ (OR) [Ar]4s ² 3d ³
Chromium	Cr	24	1s ² 2s ² 2p ⁶ 3s ² 3p ⁶ 4s ¹ 3d ⁵ (OR) [Ar]4s ¹ 3d ⁵
Manganese	Mn	25	1s ² 2s ² 2p ⁶ 3s ² 3p ⁶ 4s ² 3d ⁵ (OR) [Ar]4s ² 3d ⁵
Iron	Fe	26	1s ² 2s ² 2p ⁶ 3s ² 3p ⁶ 4s ² 3d ⁶ (OR) [Ar]4s ² 3d ⁶
Cobalt	Co	27	1s ² 2s ² 2p ⁶ 3s ² 3p ⁶ 4s ² 3d ⁷ (OR) [Ar]4s ² 3d ⁷
Nickel	Ni	28	1s ² 2s ² 2p ⁶ 3s ² 3p ⁶ 4s ² 3d ⁸ (OR) [Ar]4s ² 3d ⁸
Copper	Cu	29	1s ² 2s ² 2p ⁶ 3s ² 3p ⁶ 4s ¹ 3d ¹⁰ (OR) [Ar]4s ¹ 3d ¹⁰
Zinc	Zn	30	1s ² 2s ² 2p ⁶ 3s ² 3p ⁶ 4s ² 3d ¹⁰ (OR) [Ar]4s ² 3d ¹⁰

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