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Where Minds Pollinate

Class 11
Chemistry

Chapter 2
Atomic Structure
Handwritten Notes

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CH 02: ATOMIC STRUCTURE

History of Atomic Model

- **Dalton, 1808** First to describe atoms in a modern scientific sense. Idea of atoms. Doesn't explain electricity.
- **Thomson, 1897** Thomson's plum pudding model. Doesn't explain some of Rutherford's α-particles bounched back. Protons and electrons
- **Rutherford, 1911** Rutherford shot α-particles through gold foil; some bounced back. Why don't the electron lose energy and crash into the nucleus? Discovered the nucleus.
- **Bohr, 1913** Basis of our modern atomic model. Discovery of electron shells. Doen't explain quantum mechanics.
- **Schrodinger, 1926** Quantum Mechanics. Why are some atoms of the same element heavier? Discovers subshells. Shells are actually orbitals.
- **Chadwick, 1932** Discovers Neutrons.
- **Heisenberg, 1927** Gives 3D Model and Orbitals

Sub-atomic particles

-Electoron

- It was discovered by J.J Thomson.
- It is negatively charged sub-atomic particle with a charge $-1.6 \times 10^{-19}C$.
- It's relative charge is -1.
- It's mass is $9.1095 \times 10^{-31} kg$.
- These particles are deflected towards positive pole of electric field.

-Proton

- It was discoved by E. Rutterford.
- It is positive charged sub-atomic particle with a charge $+1.6 \times 10^{-19}C$.
- It's relative mass charge is $+1$.
- It's mass is $1.6727 \times 10^{-27} kg$.
- It is 1836 times heavier than an electron.
- These particles are deflected towards negative pole of electric field.

-Neutron

- It was discovered by J. Chadwick
- It is neutral sub-atomic particle.
- It carries no relative charge.
- It's mass is $1.6750 \times 10^{-27} kg$.
- It is 1840 times heavier than an electron.

- These particles are not deflected by electric and magnetic fields.

Behaviour of Electron, Proton and Neutron in Electric Feild

- In the presence of an electric feild, electrons and protons undergo opposing forces due to their opposite charges.
- Electrons being negatively charged, move against the electric field towards positive pole, while positively charged protons move in the direction of the electric field, towards negative pole.
- Neutrons being electrically neutral, generally experiance negligible forces and exhibit no deviation in an electric field.
- When electrons, protons and neutrons share the same velocity, their paths diverge due to the electric forces acting on electrons and protons.
- Electrons curve against the electric field, proton curve with it and neutron, having no net charge, countinue along their path with minimal deflection, their curvature also depends on the trajectory of force or velocity.

Atomic Number and Mass Number

-**Atomic Number** (also known as Proton Number, Charge Number, Identification Number) Atomic number is the number of protons in the nucleus of an atom. Since atom is neutral particle, it means that the number of electrons revolving around the nucleus are equal to the number of protons present in the nucleus. Atomic number is represented by Z.

-**Mass Number** (also known as Nucleon Number, Atomic Mass). Mass number represent the total number of protons and neutrons in the nucleus. It is represented by A. Mass number is approximately equal to the atomic mass of an atom.

∵ Atomic Number + Number of Neutron = Mass Number

$P + N = A$

Number of Protons = Number of Electrons (For a neutral atom)

Number of electrons in Cation = Atomic Number − Magnitude of Charge on Cation

Number of electrons in Anion = Atomic Number + Magnitude of Charge on Anion

Atomic and Ionic Radius

-**Atomic Radius** The average distance of nucleus from the outermost electrons is called radius of an atom. It is measure of an atom as boundary of electronic cloud is not very well defined so the term average is used.

Across the period from left to right the atomic radius decreases. Effective nuclear charge increases. Shielding effect remains constant.

In a group from top to bottom the atomic radius increases. Number of shells increases

Sheilding effect increases due to intervening electrons.

-**Ionic Radius** Ionic radius is the distance from the nucleus of an ion up to which it has an influence on its electron cloud. Ions are formed when an atom loses or gains electrons. When an atom loses an electron it forms a cation and when it gains an electron it becomes an anion. The cation are always smaller than their parent atom due to increase in effective nuclear charge and decrease in electron-electron repulsion in the valence shell due to removal of electrons. The anions are always larger than their parent atom due to increase in the electron-electron repulsion in the valence shell.

$A^{-2} > A^{-1} > A > A^{+1} > A^{+2}$

Across the period, this is debateable in the period from left to right because in period each element does not usually form ion with the same charge. The charge on the ion depends upon the valence shell electronic configuration, which changes from left to right. If we consider the same charge on each ion in periodic table from left to right in a period the trend will be the same, that is, the decrease as that of the atomic radii.

In a group from top to bottom, the trend of ionic radius is same as that of atomic radius, it goes on increasing. This due to the same charge on the ions throughout the group.

-**Importance** Atomic radius and Ionic radius effect different periodic properties as:

- Ionization energies
- Electronegativities
- Bond energies
- Bond lengths
- Oxidizing or reducing powers

Quantum Numbers

Quantum numbers are the four constants that describe the acceptable behaviour of the electron in an orbital. A set of numerical values which gives the acceptable solutions to Schrodinger's wave equation for Hydrogen atom. It describes the behaviour of electron around the nucleus.

-**Principal Quantum Numbers** Related to shell/orbit/energy level. It gives quantitative measurement. Tells the distance from nucleus. Greater number means greater size of orbit/shell. Tells energy of orbit. Represented by n. Values are non-zero, positive integers. A quantum number that describes the distance of electron with respect to the nucleus, size and the energy of the orbital is called principal quantum number.

$n = 1, 2, 3, 4, 5 \ldots\ldots$

If n=1 then its K-shell, n=2 then its L-shell, n=3 then its M-shell, n=4 then its N-shell and so on.

- The number of sub-shells in shell is equal to its "n" value.
- The number of orbitals in a shell can be calculated by "n^2" formula.
- The number of electrons in a shell can be calculated by "$2n^2$" formula.

-Azimuthal Quantum Number Related to sub-sheell. Tells energy in subshell. Represents shape of orbital. Tells nature of sub-shell. Represented by l. Always less than value of 'n'. A quantum number that gives the idea of energy and shape of subshells in a shell. The concept of existance of sub-shells in a shell, explains the splitting of spectral line in high power resolving spectrometer.

$l = 0, 1, 2, 3 \ldots\ldots$

If $l=0$ then its s-subshell, $l=1$ then its p-subshell, $l=2$, then its d-subshell, $l=3$ then its f-subshell. Subshell s has spherical shape and its nature is sharp. Subshell p has dumbbell shape and its nature is principal. Subshell d has a sausage or doub dumbell shape and its nature is diffused. Subshell f has a complicated shape and its nature is fundatamental.

- The number of orbitals in a subshell is calculated by formula "$2l+1$".
- The number of electrons in a subshell is calculated by formula "$2(2l+1)$".

-Magnetic Quantum Number Related to orbitals. Also known as "Orbital Orientation Quantum Number." Tells orbital orientation in space. Explains degeneracy of orbitals. Represented by m. Explains Zeeman's effect. This quantum number describes about number of orientations (orbitals) in a subshell. It actually explains one of the defects of Bohr (the splitting of spectral lines in magnetic field.)

$m = 0, \pm 1, \pm 2, \pm 3 \ldots\ldots$

- The number of 'm' values tells us the no. of orbitals in a sub-shell.
- The value of 'm' depends upon value of l for a sub-shell and can be calculated by $m = -l \rightarrow +l$

-Spin Quantum Number- Related to spin/self rotation of electron. Not drieved from wave equation. Invented by Goudsmit and Uhlenbeck 1925. Describe the spin of electron. Represented by S. A electron generates two opposite magnetic fields due to two opposite spins. This spin motion produces doublet line structure in emission spectrum of an atom. (Stark effect).

$S = -1/2, +1/2$

Quantum Number and Electronic Configuration

Electronic configuration means the distribution of electron around the nucleus in orbits and in turn in orbitals. A complete electronic configuration must clearly represent all the four

quantum numbers or with the help of four quantum numbers one should be able to write the complete configuration. Example:

$s=\pm\frac{1}{2}, m=0, l=0, n=2$ $\quad n=2, l=1, m=0, s=\pm\frac{1}{2}$ $\quad n=3, l=0, m=0, s=+\frac{1}{2}$

$^{11}Na = 1s^2\ 2s^2\ 2p_x^2\ 2p_y^2\ 2p_z^2\ 3s^1$

$n=1, l=0$ $\quad n=2, l=1$ $\quad n=2, l=1$
$m=0, s=\pm\frac{1}{2}$ $\quad m=+1, s=\pm\frac{1}{2}$ $\quad m=-1, s=\pm\frac{1}{2}$

Rules of Electronic Configuration

- An orbital can have maximum of two electrons.
- Maximum number of electrons in a shell $= 2n^2$.
- Maximum number of electrons in a sub-shell $= 2(2l+1)$

-n+l Rule A subshell with lowest n+l value has lowest energy and is filled first with electrons. When two or more sub-shell has the same n+l value, then fill the electron in the one that has lowest n value. $1s < 2s < 2p < 3s < 3p < 4s < 3d$.....

-Aufbau Principal Filling of electrons in sub-shells. Electrons are filled in subshells in order of increasing energy values. The energy of subshell is determined from n+l rule.
$1s < 2s < 2p < 3s < 3p < 4s < 3d$....

-Pauli Exclusion Principal Filling of electrons in orbitals. It's impossible for two electron residing in the same orbital of a poly-electron atom to have the same values of four quantum numbers. Two electrons in the same orbital should have opposite spins.

-Hund's Rule Filling of electrons in degenerate orbitals. If degenerate orbitals are available and more than one electrons are to be placed, they should be placed in separate orbitals with same spin rather than putting them in the same orbital with opposite spins. (degenerate orbitals are orbitals having same energy but different orientations) Electrons are distributed in an atom in such a way to give maximum number of unpaired electrons. Also known as "Hund's for maximum multiplicity rule".

Steps for Electronic Configuration

1. Identify the neutral atom's electronic configuration: Each neutral atom has a specific number of electrons, which can be found in the Periodic Table of Elements. For example, a neutral flourine atom has 9 electrons.
2. Determine the charge of the ion: Ion can be positively or negatively charged depending on whether they have gained or lost electrons. Positive ions (cations) have a deficit of electrons, while negative ions (anions) have an excess of electrons.
3. Write the electron configuration for the ion: For cation, start with the neutral atom's electronic

configuration and remove electrons equal to the magnitude of positive charge from outermost shell to create the ion's configuration. For anions, start with the neutral atom's electronic configuration and add electrons equal to the magnitude of negative charge in the outermost shell to create the ion's configuration.

Explanation of Electronic Configuration

- Energy of electrons and inter-electron repulsion

The relationship b/w interelectron repulsion and electronic configuration is that electrons tend to minimize repulsion by occupying their own seperate orbital, rather than sharing an orbital with another electron (Hund's rule). This is because electrons repel each other due to their identical charges and this repulsion is minimized when electrons occupy separate orbitals in the same subshell. The repulsion b/w electrons increases with the increase in the number of electrons in the same orbital, leading to a higher energy for larger orbitals.

- Orbital Energy: The energy of an orbital depends on its distance from the nucleus and the electron-electron repulsion it experiances. Orbitals with lower energies are filled before.
- Spin Pairing Energy: The energy of an orbital increases when two electrons with opposite spins occupy it. This is because the repulsion between the electrons increases when they share an orbital.

The arrangement of electrons within an atom is governed by the interplay b/w electron-electron repulsion and other ~~forces~~ factors such as electron sheilding, spin pairing energy and orbital energy.

No.	Element	Configuration	No.	Element	Configuration
1	Hydrogen	$1s^1$	14	Silicon	$[Ne]3s^2 3p_x^1 3p_y^1 3p_z^0$
2	Helium	$1s^2$	15	Phosphorus	$[Ne]3s^2 3p_x^1 3p_y^1 3p_z^1$
3	Lithium	$[He]2s^1$	16	Sulfur	$[Ne]3s^2 3p_x^2 3p_y^1 3p_z^1$
4	Beryllium	$[He]2s^2$	17	Chlorine	$[Ne]3s^2 3p_x^2 3p_y^2 3p_z^1$
5	Boron	$[He]2s^2 2p_x^1 2p_y^0 2p_z^0$	18	Argon	$[Ne]3s^2 3p_x^2 3p_y^2 3p_z^2$
6	Carbon	$[He]2s^2 2p_x^1 2p_y^1 2p_z^0$	19	Potassium	$[Ar]4s^1$
7	Nitrogen	$[He]2s^2 2p_x^1 2p_y^1 2p_z^1$	20	Calcium	$[Ar]4s^2$
8	Oxygen	$[He]2s^2 2p_x^2 2p_y^1 2p_z^1$	21	Scandium	$[Ar]4s^2 3d_{xy}^1 3d_{yz}^0 3d_{xz}^0 3d_{x^2-y^2}^0 3d_{z^2}^0$
9	Fluorine	$[He]2s^2 2p_x^2 2p_y^2 2p_z^1$	22	Titanium	$[Ar]4s^2 3d_{xy}^1 3d_{yz}^1 3d_{xz}^0 3d_{x^2-y^2}^0 3d_{z^2}^0$
10	Neon	$[He]2s^2 2p_x^2 2p_y^2 2p_z^2$	23	Vandium	$[Ar]4s^2 3d_{xy}^1 3d_{yz}^1 3d_{xz}^1 3d_{x^2-y^2}^0 3d_{z^2}^0$
11	Sodium	$[Ne]3s^1$	24	Chromium	$[Ar]4s^1 3d_{xy}^1 3d_{yz}^1 3d_{xz}^1 3d_{x^2-y^2}^1 3d_{z^2}^1$
12	Magnesium	$[Ne]3s^2$	29	Copper	$[Ar]4s^1 3d_{xy}^2 3d_{yz}^2 3d_{xz}^2 3d_{x^2-y^2}^2 3d_{z^2}^2$
13	Aluminium	$[Ne]3s^2 3p_x^1 3p_y^0 3p_z^0$	36	Krypton	$[Ar]4s^2 3d^{10} 4p_x^2 4p_y^2 4p_z^2$

Shapes of Orbitals

The shapes of orbitals can be explained on the basis of azimuthal and magnetic quantum number. Orbital is a region with 95% probability of finding electrons. Node/Nodal Plane/Nodar Surface is a region where probability of finding electrons is 0 b/w two orbitals.

-Shape of s-orbital Only one value of magnetic quantum number i.e m=0, so only one orbital. It is spherical in shape. Represented by a circle. With the value of 'n', its size increases and distance from nucleus also increases.

-Shape of p-orbital There are 3 values of magnetic quantum number of p-shell, m=-1,0,+1. Three orientations in space (p_x, p_y, p_z). These three orbitals are perpendicular to each other. Directional in nature. It gives difinite shape to the molecules. It is dubbell in shape. Size increases with value of 'n'.

-Shape of d-orbital There are 5 values of magnetic quantum number of d-shell, m=-2,-1,0,+1,+2. Five orientations in space (d_{xy}, d_{xz}, d_{yz}, $d_{x^2-y^2}$, d_{z^2}). d_{xy}, d_{xz}, d_{yz} and $d_{x^2-y^2}$ have four lobes each double dumbell/sausage/clover leaf, while d_{z^2} have two lobes and a doughut at the center doughut/dumb-bell with collar. In the absence of magnetic field, all the five d-orbitals are degenrate.

-Shape of f-orbital Shape of f-orbitals are complicated.

Ionization Energy

The minimum energy needed to remove the outermost electron (most losely bonded electron) from the gaseous isolated atom. Atom is needed to be in the gaseous state to avoid the influence of other factors like heat of fusion, bond disscociation energy and heats of vapourization.

$$Mg_{(g)} \longrightarrow \underset{IE_1 = 738 kJ mol^{-1}}{Mg^{+}_{(g)}} \longrightarrow Mg^{+2}_{(g)} \longrightarrow Mg^{+3}_{(g)}$$

- Always endothermic
- Measure of stability of an atom
- Predict reactivity of an atom.

-Periodic Trend

Along Periods: Ionization energy increases from left to right in a period with slight anomalies. With each step from left to right in the periodic table, the number of protons increases which strengthen the attraction of nucleus on the electrons. From left to right in main group elements sheilding effect remains constant, so there is no effect on the ionization energy values in this respect. Hence, with the increase in effective nuclear charge along period, ionization energy of elements also increases. Atomic radius decreses from left to right which brings the electrons near to the nucleus thus the attraction is increased and so does the ionization energy.

Down the group: In a group from top to bottom, the ionization energy decreases. Down the group, with the increase in the number of shells, the atomic size increases which result in decrease in nuclear attraction for the valence electrons and ionization energy decreases With the increase in number of shells down the group, the shielding effect increases and it becomes easier to remove the valunce electron.

- Factors influencing ionization energy

Nuclear Charge: As the nuclear charge increases moving from left to right in periodic table the attraction on the outermost electron also increase which in turn will increase the ionization energy. This is just according to the Coloumb's law.

Atomic Radii: Moving from left to right in the table decreases the radii which stengthens the attraction of nucleus on electrons, increasing the ionization energy. From top to bottom size increases and ionization energy decreases.

Shielding effect: As you move down a group, the number of electron shell increases. The inner electron shells act as a sheild, reducing the effective nuclear charge felt by the outer electrons. This sheilding effect makes it easier to remove outer electrons, leading to decrease in ionization energy down a group. From left to right sheilding effect remains constant and poses no effect on inoization energy.

Spin Pair Repulsion: When electron are paired in half filled p ordibat of partially filled substell there is electron pair repulsion which causes the energy of electron to increase. Increased energy makes the electron easier to remove and therefore the ionization energy decreases.

Mass Spectrometry

Technique used to determine • the exact relative isotopic atomic mass. • relative abundance of isotopes. • mass-to-charge ratio of ions. • structure of a molecule.

- Types of mass spectrometer

Aston's mass spectrometer: Identify the isotopes of an element based on their atomic mass. Identify the isotopes of the elements in gaseous state.

Dempster's mass spectrometer: Identify the isotopes of an element based on their atomic mass. Identify the isotopes of the elements in solid state.

Modern mass spectrometer: Identify the isotopes of the elements in gas, liquid and solid state. Contains two additional components (Amplifier, Recorder)

- Working of Spectrometer

Ionization: The sample is introduced into the ion source where it is ionized. This process can involve bombarding the sample with high-energy electrons, introducing it to high-voltage field, or using

a laser to vaporize it.

Ion Seperation: The resulting ions are then accelerated and directed into the mass analyzer. The mass analyzer separates ions based on their m/z ratio, allowing ions of different masses to be focused and detected at different times.

Detection: As the ions exit the mass analyzer, they hit the detector. The detector records the time it takes for each ion to reach it, and this data is used to calcute the m/z ratio of each ion.

Data Analysis: The information collected from the dector is used to construct a mass spectrum. The x-axis of the spectrum represents the m/z ratio, while the y-axis represents the abundence of ions at each m/z ratio. Peaks in the spectrum correspond to different ions present in the sample, with their positions revealing their masses.

- **Applications:**
  - Relative abundence of isotopes of an element.
  - Identifying of unknown compounds.
  - Quantifying the amounts of specific substance.
  - Elucidating molecular structures.
  - Studying biomolecules like proteins and nucliec acids etc.
  - Determining the average atomic mass of an element.

$$\text{Average atomic mass} = \frac{(\text{Mass No.} \times \text{Relative abundance})_1 + (\text{Mass No.} \times \text{Relative abundence})_2 \ldots}{100}$$

$$= \frac{(\text{RIM} \times \text{RA})_1 + (\text{RIM} \times \text{RA})_2}{100}$$

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