Q.10 How does the reactivity of Group 1 and Group 17 elements change down the group?

Ans. In Group 1, reactivity of elements increases down the group because the outermost electron is more easily lost. In Group 17, reactivity of elements decreases down the group as gaining an electron becomes harder.

Q.11 How do transition metals differ from s-block elements?

Ans. The transition metals differ from s-block elements because of following aspects:

- Transition metals can form multiple oxidation states.
- They often form colored compounds.
- They act as catalysts.
- They involve the filling of d-orbitals.

Q.12 Why do non-metals tend to gain electrons while metals tend to lose them?

Ans. The non-metals have high electronegativity and nearly full valence shells, so that is why, they tend to gain electrons. On the other hand, metals have low ionization energy and few valence electrons, that is why, they lose them easily.

SELF-ASSESSMENT Chapter # 01

Total Mark: 30

Q.1 Encircle the correct option. **(1 × 6 = 6)**

(i) Which of the following elements is not a member of the chalcogen family?
(A) Oxygen (O) (B) Sulfur (S) (C) Selenium (Se) (D) Bromine (Br)

(ii) Non-metals are present in which block of periodic table?
(A) s-block (B) p-block (C) d-block (D) f-block

(iii) Which of the following has the highest electron affinity?
(A) Fluorine (B) Chlorine (C) Bromine (D) Iodine

(iv) Among the following members of group 14 which is a non-metal?
(A) C (B) Si (C) Ge (D) Sn

(v) The oxides of electropositive elements are:
(A) Acidic (B) Basic (C) Amphoteric (D) Neutral

(vi) Oxidation number of Al in Al_2O_3 is:
(A) +2 (B) +3 (C) +4 (D) +5

Q.2 Write short answers of the following questions. **(2 × 8 = 16)**

(i) Why are the elements in groups 1 and 2 known as s-block elements?
(ii) How does electron affinity varies in a group of the periodic table?
(iii) Using your knowledge of Period 3 elements, predict and explain the relative sizes of the atomic radii of lithium and fluorine.
(iv) Explain with reasoning following facts about ionization energy 1^{st} ionization energy of Boron is lesser than Beryllium.
(v) What is the nature of oxides and hydroxides of Na and Mg?
(vi) ZnO reacts with HCl to give $ZnCl_2$ and with NaOH to give Na_2ZnO_2. Give equations and also predict the type of this oxide?
(vii) Discuss any two factors affecting electronegativity.
(viii) What is the role of Shielding Effect on Ionization Energy?

Q.3 Extensive Questions. **(2 × 4 = 8)**

(a) Define 1^{st}, 2^{nd} and 2^{nd} Ionization Energy with one example each. Also discuss periodic trends in ionization energy.
(b) Write down the reactions of Na and Mg with water, Oxygen and Chlorine (equations only).

Chapter 02 ATOMIC STRUCTURE

Student Learning Outcomes

After studying this chapter, students will be able to:

- Describe protons, neutrons, and electrons in terms of their relative charge and relative masses. **(Understanding)**
- Recognize that the terms atomic and proton number represent the same concept. **(Understanding)**
- Recognize that the terms mass and nucleon nuclear represent the same concept. **(Understanding)**
- Explain the change in atomic and ionic radius across a period and down a group. **(Understanding)**
- Describe the behaviour of beams of protons, neutrons and electrons moving at the same velocity in an electric field. **(Understanding)**
- Determine the number of protons, neutrons, and electrons present in both atoms and ions given atomic or proton number, mass/or nucleon number and charge. **(Knowledge)**
- Relate Quantum Numbers to electronic distribution of elements. **(Understanding)**
- Account for the variation in successive ionization energies of an element. **(Understanding)**
- Define terms related to electronic configuration (some examples include: shells, subshells, orbitals, principal quantum number (n), ground state). **(Knowledge)**
- Describe the order of increasing energy of the sub-shells (s, p, d, and f). **(Understanding)**
- Describe that, each atomic shell and sub-shell are further divided into degenerate orbitals having the same energy. **(Understanding)**
- Apply Aufbau principle, Pauli's exclusion principle and Hund's rule to write the electronic configuration of elements. **(Application)**
- Describe the number of orbitals making up s, p, d, and f sub-shells, and the number of electrons that can fill s, p, d, and f sub-shells. **(Understanding)**
- Describe the shapes of s, p, and d orbitals. **(Understanding)**
- Determine the electronic configuration of elements and their ions with proton numbers. **(Knowledge)**
- Some examples include:
  a. simple configuration e.g., 2,8
  b. Sub-shells e.g., $1s^2, 2s^2, 2p^6, 3s^1$
  c. students should be able to determine both of these from periodic table and are not required to memorize these.
  d. Students should understand that chemical properties of an atom are governed by valence electrons.
- Explain the electronic configurations to include the number of electrons in each shell, subshell and orbitals. **(Understanding)**
- Explain the electronic configurations in terms of energy of the electrons and inter-electron repulsion. **(Understanding)**
- (Determine the electronic configuration of atoms and ions given the proton or electron number and charge. **(Understanding)**

- Describe free radical as a species with one or more unpaired electrons. **(Understanding)**
- Illustrate the importance of electronic configurations and development of new materials for electronic devices. (For example, semiconductors such as silicon has a specific electronic configuration that makes them ideal for their use in electronic devices) **(Understanding)**
- Deduce the electronic configurations of elements using successive ionization energy data. **(Application)**
- Deduce the position of an element in the periodic table using successive ionization energy data. **(Application)**
- Explain that ionization energies are due to the attraction between the nucleus and the outer electrons. **(Understanding)**
- Explain how ionization energy helps account for the trends across the period and down a group of the periodic table. **(Understanding)**
- Explain the factors influencing the ionization energies of elements in terms of nuclear charge, atomic/ionic radius, shielding by inner shells and sub-shells and spin pair repulsion. **(Understanding)**

ATOMIC NUMBER, PROTON NUMBER AND NUCLEON NUMBER; IDENTITY OF AN ELEMENT

Atomic Number (Z)

"Atomic number is the number of proton in the nucleus of an atom".

In 1913, Moseley observed that when different elements were bombarded with cathode rays, the X-rays of some characteristic frequencies were produced. It was found that the **"the square root of the frequency of the X-rays was directly proportional to the atomic number of an element Z".**

$$\sqrt{\text{frequency}\,(v)} \propto Z$$

- Moseley concluded that this number, i.e. the atomic number Z was a fundamental property of an element.
- It is also called proton number.

Nucleon Number

"The number of protons and neutrons in the nucleus of an atom is collectively called its nucleon number (A), also called mass number".

Atomic number is related to the mass number by the following equation

$$A = Z + N$$

Example: An atom of an element X having atomic number Z and mass number A is described as ${}^{A}_{Z}X$, e.g. ${}^{27}_{13}A\ell$. Number of neutrons in an atom can be calculated as

$$N = A - Z$$

For example, ${}^{27}_{13}A\ell$

Atomic number/proton number $(Z) = 13$

Mass number/nucleon number $(A) = 27$

$$N = 27 - 13 = 14$$

Similarly, the number of electrons, protons, and neutrons can be justified for an ion as in the following example:

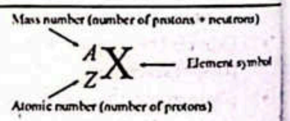
${}^{27}_{13}A\ell$ atom loses three electrons to form $A\ell^{3+}$ then, For $A\ell^{3+}$

- No. of protons = 13
- No. of neutrons = 14
- No of electrons = 13 − 3 = 10

Similarly, ${}^{35}_{17}C\ell$ gains an electron to form $C\ell^-$ ion, then, For $C\ell^-$

Rack Your Brain!

1. The total number of fundamental particles in an atom of Carbon − 14 is:
(A) 6 (B) 8
(C) 14 (D) 20



- No. of protons = 17
- No. of neutrons = 18
- No of electrons = 17 + 1 = 18

In the cases where electron gain happens by the neutral atoms, say ${}^{16}_{8}O$ to ${}_{8}O^{2-}$, ${}^{31}_{15}P$ to ${}_{15}P^{3-}$ and ${}^{32}_{16}S$ to ${}_{16}S^{2-}$, the number of neutrons, protons and electrons are as follows:

Table: Number of protons, electrons and neutrons in different ions

Species	Neutrons	Protons	Electrons
O^{2-}	8	8	10
S^{2-}	16	16	18
P^{3-}	16	15	18

Thus the atomic number and proton number represent the same concept.

EFFECT OF ELECTRIC FIELD ON FUNDAMENTAL PARTICLES

The behaviour of particles in an electric field depends upon their mass and charge. If we allow the beams of electrons, protons and neutrons to pass one by one at the same speed through an electric field, they show their behaviour as follows.

1. Neutrons being neutral are not deflected but travel in a straight path perpendicular to the direction of electric field.
2. Protons being positively charged are deflected towards the negative plate.
3. Electrons being negatively charged are deflected towards the positive plate, to greater extent since they are $\frac{1}{1836}$ times lighter than protons.

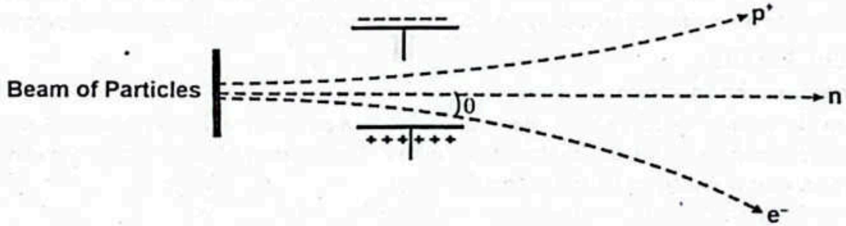


Figure: Behaviour of proton, electron and neutron in the electric field

The amount of deviation from its original direction of movement is measured in two ways.

(i) Angle of deflection $\propto \frac{\text{charge}}{\text{mass}}$

(ii) Radius of deflection $\propto \frac{\text{mass}}{\text{charge}}$

This is possible if we imagine that after deflection, the particle moves in a circular path. Hence, *the factors affecting the radius of deflection are reciprocal to that for the angle of deflection.*

Rack Your Brain!

2. Cathode rays are negatively charged. Why?

Properties of Fundamental Particles

The Table shows the properties of three fundamental particles electron, proton and neutron present in an atom.

Table: Properties of three fundamental particles

Particle	Charge (coulomb)	Relative charge	Mass (kg)	Mass (amu)
Proton	$+1.6022\times10^{-19}$	+1	1.6726×10^{-27}	1.0073
Neutron	0	0	1.6750×10^{-27}	1.0087
Electron	-1.6022×10^{-19}	-1	9.1095×10^{-31}	5.4858×10^{-4}

QUICK CHECK 2.1

a) Calculate the number of neutrons in the following elements.

(I) $^{39}_{19}K$ (II) $^{35}_{17}C\ell$ (III) $^{40}_{18}Ar$

Ans.

Number of Neutrons in:		
(I) $^{39}_{19}K$	(II) $^{35}_{17}C\ell$	(III) $^{40}_{18}Ar$
Mass number = A = 39 Number of Protons = Z = 13 Number of Neutrons = N = A − Z = 39 − 13 = 26	Mass number = A = 35 Number of Protons = Z = 17 Number of Neutrons = N = A − Z =35 − 17 = 18	Mass number = A = 40 Number of protons = Z = 18 Number of Neutron = N = A − Z = 40 − 18 = 22

b) Which of electron, proton and neutron is deflected the most in the magnetic field?

Ans. Electron is deflected the most because it is charged and has a very small mass.
Proton is deflected less because it is charged but much heavier.
Neutron is not deflected at all because it has no charge.

EXPERIMENTAL EVIDENCES FOR THE ELECTRONIC CONFIGURATION

The modern theory of electronic structure takes its origin from the Bohr Model of atom. ***Evidence for this and later models of the atoms derives principally from two sources; atomic spectra and ionization energies.***

➲ Atomic Spectra

➤ **Atomic Emission Spectrum:**

"When an element in its gaseous state is heated to high temperatures or subjected to electrical discharge, radiation of certain wavelengths is emitted. The spectrum of this radiation contains coloured lines and is called atomic emission spectrum".

The atomic emission spectrum of hydrogen is shown in Figure (a).

➤ **Atomic Absorption Spectrum:**

"When a beam of white light is passed through a gaseous sample of an element in cold state, certain wavelengths are absorbed. The wavelengths of the white light that has been absorbed by the atoms show up as dark lines on the spectrum. The spectrum of this radiation is called an atomic absorption spectrum".

The atomic absorption spectrum of hydrogen is shown in Figure (b).

NOTE: The wavelengths of the dark lines in the absorption spectrum are exactly the same as those of coloured lines in the emission spectrum.

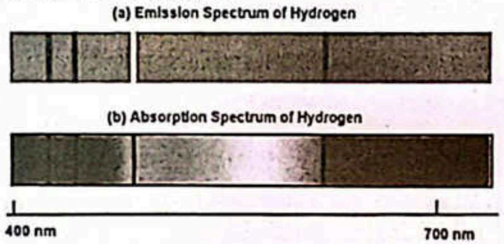


Figure: (a) atomic emission spectrum of hydrogen (b) atomic absorption spectrum of hydrogen

- Each element has a unique arrangement of electrons and thus a unique range of fixed energy levels.
- The wavelengths and frequencies of the radiation absorbed or emitted when electrons jump from one energy level to another must also be unique.
- This uniqueness convinces us to conclude that every element has its own characteristic spectrum. Therefore, every element is identified by its characteristic spectrum.
- The atomic spectra are the finger prints of the elements. Figure shows the emission spectra of some elements.

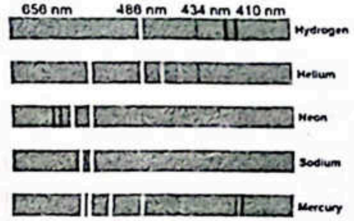


Figure: Spectral series of various elements as plotted by a spectrometer

(Exercise L.Q.5)

Q. What do you mean by successive ionization energies? How the electronic shell structure of magnesium (Mg) is derived from the successive ionization energies?

➲ Ionization Energy and Energy Levels (Electronic Shells)

A major difference between electrons in different types of shells is their energy. We can investigate the electronic configuration of the atoms by measuring experimentally the energies of the electrons within them. This can be done by measuring ionization energies.

Ionization energies are used to investigate the electronic configurations of elements in two ways.

i. Successive ionization energies of the same element
ii. First ionization energies for different elements

i) Successive Ionization Energies of the Same Element

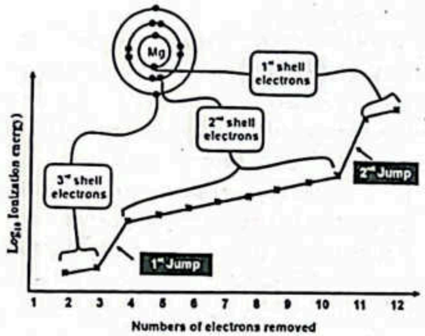
We can look at an atom of a particular element and measure the energy required to remove each of its electrons, one by one.

$$X \longrightarrow X^{+} + e^{-} \quad \Delta HI_1$$
$$X^{+} \longrightarrow X^{2+} + e^{-} \quad \Delta HI_2$$
$$X^{2+} \longrightarrow X^{3+} + e^{-} \quad \Delta HI_3$$

We can continue to remove electrons from an atom until only the nucleus is left. We call this sequence of ionization energies, successive ionization energies. The successive ionization energies show clearly the arrangement of electrons in shells around the nucleus.

Example: If we take the magnesium atom as an example, and measure the energy required to remove successively the first electron, the second, the third, and so on. We obtain a graph when the ionization energies values are plotted against number of electrons as in Figure.

$$Mg_{(g)} \longrightarrow Mg^{+}_{(g)} + e^{-} \quad \Delta H_{i1} = +738 kJ\ mol^{-1}$$
$$Mg_{(g)} \longrightarrow Mg^{2+}_{(g)} + e^{-} \quad \Delta H_{i2} = +1450 kJ\ mol^{-1}$$
$$Mg^{2+}_{(g)} \longrightarrow Mg^{3+}_{(g)} + e^{-} \quad \Delta H_{i3} = +7730 kJ\ mol^{-1}$$



L/Q. Electrons in Magnesium atoms exist in three shells. Prove with a graph.

Figure: A plot of the successive ionization energies of Mg

> **Graph Depicting Successive Ionization Energies:**

- This plot shows that *successive ionization energies increase when we move from the valence shell t the inner shells.*
- First two electrons are removed from the outermost shell and require lower energy for their removal.
- A very large increase occurs when the third electron is removed. This is because when two electrons the outer shell have been removed, the next has to be removed from the shell that is very much clos to the nucleus. The next seven electrons are removed successively from the second shell and a gradu increase in ionization energy is observed.
- A similar but much more enormous jump occurs when the eleventh and twelfth electrons are removed.
- These electrons are removed from the first, innermost shell, right next to the nucleus. Hence, over a we observe two large jumps in the successive ionization energies. These two large jumps in the seri of successive ionization energies are very good evidence that the electron in the magnesium aton exist in three different shells.

II) First Ionization Energies of Different Elements

The second way in which ionization energies show us the details of electronic configuration is to look how the first ionization energies of elements vary with atomic numbers. The following figure shows a pl for the first 88 elements.

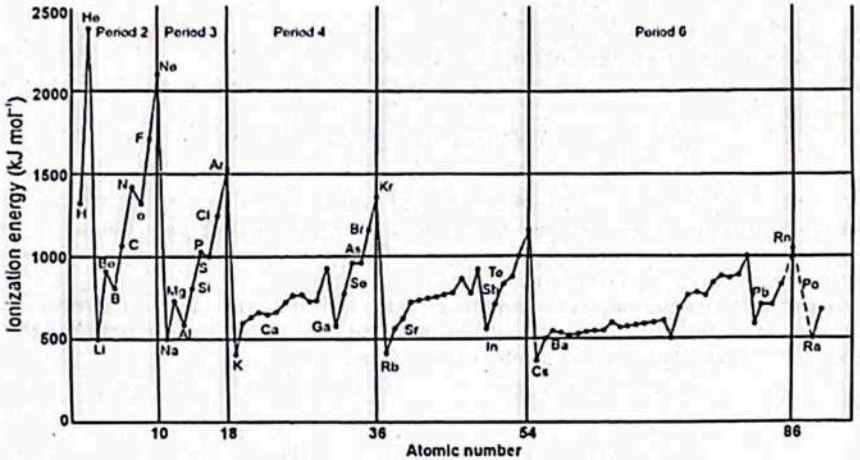


Figure: A plot of the ionization energies of first 88 elements against atomic number

This graph tells us the following:

- ***All ionization energies are strongly endothermic;*** it takes energy to separate an electron from an atom.
- **Down the Group:** As we go down a particular group, e.g., from Helium to Neon to argon, or fro Lithium to Sodium to potassium, ionization energies decrease. The larger the atom, the easier is separate an electron from it. ***Actually, down the group, number of shells increases, hold of nucleus t the valence electrons decreases, hence removal of electrons becomes easier.***
- **Along a Period:** ***The ionization energies generally increase on going across a period.*** The group elements, the alkali metals, have the lowest ionization energy within each period, and the noble gas have the highest. It is due to the reason that across the period shell number remains same. As t proton number increases, electrons are added in the same shell. Therefore, nucleus attracts t valence electrons more strongly. As a result, ionization energy increases across the period.

QUICK CHECK 2.2

a) Write equations that describe:

I. 1st ionization energy of calcium

Ans. $Ca_{(g)} \longrightarrow Ca^{+}$ $\quad \Delta H_1 = kJ/mol$

II. 3rd ionization energy of potassium

Ans. $K^{2+}_{(g)} \longrightarrow K^{3+} + 1e$ $\quad \Delta H_3 = kJ/mol$

III. 2nd ionization energy of lithium

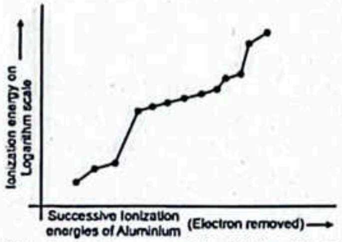
Ans. $Li^{+1}_{(g)} \longrightarrow Li^{+} + 1e^{-}$ $\quad \Delta H_2 = kJ/mol$

IV. 5th ionization energy of sulphur.

Ans. The 5th ionization energy of Sulphur is 7004.3 kJ/mol.

b) For the element aluminium (Z = 13), draw a sketch graph between the log 10 of the successive ionization energies (y-axis) against the number of electrons removed (x-axis).

Ans.



c) The first ΔH_{i1} and the second ΔH_{i2} ionization energies (kJ / mol) of a few elements are given in table.

Element	ΔH_{i1}	ΔH_{i2}
I	2372	5251
II	520	7300
III	900	1760
IV	1680	3380

Which of the above element is likely to be:

I. a reactive metal,

Ans.

Element	ΔH_{i1}	ΔH_{i2}
II	520	7300

II. a reactive non-metal,

Ans.

Element	ΔH_{i1}	ΔH_{i2}
IV	1680	3380

III. a noble gas

Ans.

Element	ΔH_{i1}	ΔH_{i2}
I	2372	5251

IV. a metal that forms a stable binary halide of the formula AX_2 (X = halogen).

Ans.

Element	ΔH_{i1}	ΔH_{i2}
III	900	1760

QUANTUM NUMBERS

(Exercise LQ)

Q. What are quantum numbers? Describe briefly principal and spin quantum numbers.

- The Bohr model was a one-dimensional model that used one quantum number to describe the distribution of electrons in the atom.
- ***The only important information was the size and energy of the orbit,*** which was described by the Principal (n) quantum number. Since Schrodinger's model allowed the electron to occupy three-dimensional space, therefore, it required three coordinates, or three quantum numbers, to describe the orbitals in which electrons can be found.
- ***The three quantum numbers that come from Schrödinger's wave equations are the principal (n), angular (l), and magnetic (m) quantum numbers.***
- ***These quantum numbers describe the size, shape, and orientation in space of the orbitals in an atom.***

> **Rack Your Brain!**
>
> 3. Quantum number values for '3d' orbital will be:
> (A) n = 3, l = 0 (B) n = 3, l = 1
> (C) n = 3, l = 2 (D) n = 3, l = 3

> **Rack Your Brain!**
>
> 4. Quantum number value for 2s orbitals are:
> (A) n = 2, l = 1 (B) n = 1, l = 2
> (C) n = 1, l = 0 (D) n = 2, l = 0

Principal Quantum Number (n)

- The principal quantum number, n, can have positive integral values 1,2,3,4... designated by K, L, M, N..., and it corresponds the quantum number (number of orbit) in Bohr's model of the hydrogen atom.
- ***This quantum number, n, describes the size and energy of the orbital.***
- The collection of orbitals with the same values of n is called an electron shell.
- The larger 'n' is, the greater the average distance of an electron in the orbital from the nucleus and therefore the larger the orbital.
- ***An increase in 'n' also means that the electron has a higher energy and is therefore less tightly bound to the nucleus.***
- The principal Quantum number, n, can also be used to calculate the maximum number of electrons in a shell by the formula $2n^2$.
- Therefore shells K, L, M and N can accommodate maximum electrons. 2, 8, 18, 32 respectively.

> **Rack Your Brain!**
>
> 5. What is the value of (n + l) for the 3d sub-shell?
> (A) 3 (B) 4
> (C) 5 (D) 6

> **Rack Your Brain!**
>
> 6. (n + l) value for 5s orbital will be:
> (A) 3 (B) 5
> (C) 7 (D) 9

(Exercise LQ)

Q. Draw the shapes of s, p and d-orbitals. Justify these by keeping in view the azimuthal and magnetic quantum numbers.

Azimuthal Quantum Number (l)

- Azimuthal quantum number also called Angular Momentum Quantum Number, l, can have integral values 0 to (n − 1) for each value of n.
- ***This quantum number describes the shape of the orbital.***
- The values of 'l' are integers that depend on the value of the principal quantum number.
  - If n = 1, there is only one possible value of 'l', i.e., l = 0 (n − 1, where n = 1).
  - If n = 2, there are two values of 'l' i.e. 0 and l.
  - If n = 3 there are, three values of 'l' i.e. 0,1 and 2.
  - If n = 4, there are four values of 'l', i.e. 0,1,2, and 3.

> **Rack Your Brain!**
>
> 7. For azimuthal quantum number l = 3, calculate the total values of magnetic quantum number (m).

- ***The values of 'l' are designated by the letters s,p,d, and f, with which stand for sharp, principal, diffused and fundamental, respectively.*** These are the spectral terms used to describe certain features of spectral lines.
- **Subshell:** The set of orbitals that have the same n and l values is called a subshell. The number of electrons in a subshell can be calculated by the formula **2(2l + 1)** as given in the Table.

Table: Shapes of orbital

Value of l	0	1	2	3
Orbital designation	s	p	d	f
shape of orbital	spherical	polar (dumb bell)	cloverleaf (double dumb bell)	complicated
No. of electrons in a subshell, 2(2l+1)	2	6	10	14

- The number of subshells in a shell is equal to its shell number. For example 1st, 2nd, 3rd, and 4th shells have one, two, three and four subshells respectively.

Table: Relationship between n, l and subshells

Shell	Principal Quantum number n	(Azimuthal) Quantum Number (l)	Subshells	No. of subshells in a shell
K	1	0	1s	1
L	2	0 1	2s 2p	2
M	3	0 1 2	3s 3p 3d	3
N	4	0 1 2 3	4s 4p 4d 4f	4

Magnetic Quantum Number (m) (Orbital Orientation Quantum Number)

- The magnetic quantum number 'm' describes the orientation of an orbital in space.
- Within a subshell, the value of m depends on the value of l. For a certain value of l there are (2l + 1) integral values of m as follows:

$$-l \ldots\ldots 0 \ldots\ldots +l$$

- The values of m indicate the number of orbitals in a subshell.
- If l = 0, (s-subshell) there is only one possible value of m, i.e. 0. It means s-subshell has only 1 orbital.
- If l = 1, (p-subshells) there are three values of m; −1, 0 and +1. It means p-subshells has three orbitals.
- If l = 2, (d-subshell), there are five values of m, namely, −2, −1, 0, +1 and +2. It means d-subshells have 5 orbitals.
- If l = 3, (f-subshell) there are seven values of m: i.e. −3, −2, −1, 0, +1, +2, +3. It means f -subshells have 7 orbitals.

> **Did You Know?**
>
> Splitting of small fine lines in the presence of magnetic field and there three dimensional orientation in space indicate the presence of orbitals in subshells.

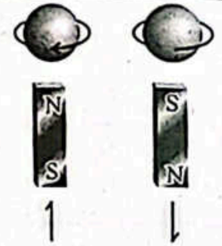
- **Degenerate Orbitals:** ***Orbitals of the same subshell have same energy and are called degenerate orbitals.*** These degenerate orbitals are differentiated from each other in the presences of magnetic field, hence the name of this quantum number, i.e. magnetic quantum number. The relationship between the magnetic quantum numbers is provided in Table.

Table: Relationship between ℓ and m

Subshell	Azimuthal / angular Quantum number (ℓ)	Magnetic Quantum number (m) $-\ell$ ....0........ $+\ell$	Number of degenerate orbitals $(2\ell+1)$
s	0	0	One orbital
p	1	−1 0 +1	Three degenerate p-orbitals
d	2	+2 +1 −1 −2	Five degenerate d-orbitals
f	3	+3 +2 +1 0 −1 −2 −3	Seven degenerate f-orbitals

Spin Quantum Number (s)

- ***Electrons are thought of spinning around their own axes (as the Earth does).***
- According to electromagnetic theory, a spinning charge generates a magnetic field.
- It is this motion that causes an electron to behave like a magnet. Figure shows the two possible spinning motions of an electron. One is clockwise and the other is anticlockwise.
- To take the electron spin into account, it is necessary to introduce a fourth quantum number called the electron spin quantum number (s).
- Its values are $+\frac{1}{2}$ and $-\frac{1}{2}$.
- The anti-clockwise spin is represented by an arrow (↑) pointing upwards, while the clockwise spin is represented by an arrow (↓) pointing downwards.
- Each orbital can accommodate at the most two electrons provided the two electrons have opposite spins.
- Thus it takes three quantum numbers to describe an orbital but forth quantum number to differentiate between the two electrons that can occupy an orbital.



(a) (b)
Figure: (a) clockwise (b) counterclockwise spins of an electron.

Did You Know?
In the nth principal quantum number, there are n subshells consisting of n^2 orbitals with a maximum number of $2n^2$ electrons.

QUICK CHECK 2.3

a) What information about an electron in an atom can be obtained from:

i. Principal Quantum Number(n)
- The different energy levels in Bohr's atom are represented by 'n'. This is called principal quantum number by Schrodinger.
- Its value is non-zero, positive integers upto infinity.

  n = 1, 2, 3, 4, ... (n ≠ 0, −ve, fractional)
- The value of 'n' represents the shell or energy level in which the electron revolves around the nucleus.

n	1	2	3	4
Shell	K	L	M	N

- These value of 'n' tells us about the radius of orbit.

ii. Azimuthal Quantum Number (ℓ)
- The presence of several fine lines in an individual line spectrum can be explained in term of Azimuthal quantum number. Azimuthal quantum number is also known as angular momentum or secondary or subsidiary quantum number.
- It is represented by 'ℓ'.
- Its values are $\ell = 0, 1, 2, 3, ... (n-1)$
- Its value depends upon the value of n.

iii. Magnetic Quantum Number (m)
To explain one of the defects of Bohr's model i.e. Zeeman effect (splitting of spectral lines due to strong magnetic field) a third quantum number called magnetic quantum number (m) has been proposed.
- This quantum no. is represented by 'm'.
- Where m = 0, ±1, ±2, ±3

iv. Spin Quantum Number (s)
- The doublet line structure of line spectrum can be explained by spin Quantum number.
- Alkali metals have one electron in their outermost shell. We can record their emission spectra, when the outermost electron jumps from an excited state to a ground state. When the spectra are observed by means of high resolving power spectrometer, each line in the spectrum is found to consist of pair of lines, this is called doublet line structure.

b) For an electron(s):

i. If $n=2$ and $\ell=1$, how many orientations in space are possible?
Ans. 2p has 3 orientations i.e. p_x, p_y, p_z

ii. If $n=3$ and $\ell=2$, which shell and subshell does the electron belong to?
Ans. 3d
Shell number 3 (M-shell)
Subshell = d

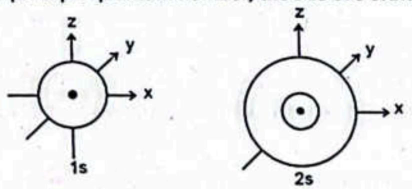
iii. If $\ell=2$, find all possible values of m and maximum number of electrons for m.
Ans. d subshell
It has five orientation m = +2, +1, 0, −1, −2.

SHAPES OF ATOMIC ORBITALS

Atomic Orbital
An atomic orbital is defined as the three dimensional region in space around the nucleus in which the probability of finding the electron is maximum.
Let us discuss the different orbitals one by one.

s-orbital

- The shape of an 's' orbital is spherical.
- The electronic density around the nucleus in an s orbital is uniformly distributed in all directions.
- With the increase in the principal quantum number, the size of s orbital also becomes larger.



(a) n = 1, ℓ = 0, m = 0 (b) n = 2, ℓ = 0, m = 0
Figure: The boundary surface for, (a) 1s (b) 2 s

p-orbitals

- The distribution of electron density for a 2p orbital is shown in Figure.

- The electron density is not distributed in a spherically symmetric fashion as in an *s* orbital. Rather, a p orbital has two lobes on any of the axis.
- The p orbitals are named as p_x, p_y and p_z, accordingly to their axes.

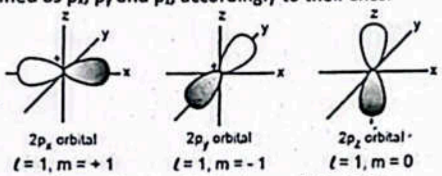


Figure: The 2p orbitals shapes of 2P orbitals

d and f orbitals

- In a given shell, 'd' orbitals have different shapes and orientations in space.
- The d_{xy}, d_{xz} and d_{yz} lie in the xy, xz and yz planes, respectively.
- The lobes of the $d_{x^2-y^2}$ lie along the x and y axes. The d_{z^2} orbital has two lobes along the z -axis and a "doughnut" in the xy plane.
- The shapes for the five d orbitals ($l = 2$) are shown in Figure.

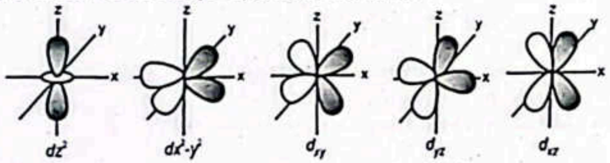


Figure: The shapes of the five 3d orbitals

An *f* subshell has seven orientations in space, i.e. there are seven *f* orbitals. However, the shapes of *f* orbitals are very complicated.

QUICK CHECK 2.4

a) What does an orbital represent according to the wave mechanical model of atom?

Ans. According to the wave mechanical model of atom, an orbital represents a region of space around the nucleus where there is high probability of finding an electron. It is a 3-D wave function that describes the electrons state and energy.

b) There are three orientations of p-orbital due to three values of magnetic quantum number. Justify it.

Ans. For p-orbital value of $l = 0$, $m = 0, +1, -1$

So there are three orientations of p-orbital.

ELECTRONIC CONFIGURATION

"Electronic configuration is the distribution of electrons among available shells, subshells, or orbitals of an atom or ion".

- In case of subshells, the electronic configuration is described by a notation that lists the subshell symbols, one after the other.
- Each symbol has a superscript on the right. This gives the number of electrons in the subshell. For example, the configuration of ${}^{9}_{4}Be$ atom with two electrons in the ' 1s ' subshell and two electrons in the ' 2s ' subshell is written $1s^2 2s^2$.
- Each group of orbitals in a subshell is labeled by its subshell notation.
- An electron in an orbital is shown by an arrow. The arrow points upward, when $s = +1/2$ and downward when $s = -1/2$. The orbital diagram of boron (${}^{11}_{5}B$) is as follows

$${}^{11}_{5}B = 1s^2, 2s^2, 2px^1, 2py^0, 2pz^0$$

Distribution of Electrons in Shells

- The electronic configuration of an atom describes the distribution of electrons in its atomic shells.
- The shells, denoted as K, L, M, N, and so on, correspond to the principal quantum number (n) of the orbitals.
- Shell capacities each shell has a specific capacity for electrons:
  - **K shell (n=1): 2 electrons maximum (1 s orbital)**
  - **L shell (n=2): 8 electrons maximum (2 s and 2 p orbitals)**
  - **M shell (n=3): 18 electrons maximum (3s, 3p, and 3d orbitals)**
  - **N shell (n=4): 32 electrons maximum (4s, 4p, 4d, and 4 f orbitals)**

Rack Your Brain!

8. Calculate the number of electrons in s, p, d and f sub shells from the formula and write separately.

For example:

- **Hydrogen (H):** $1s^1$ (K shell)
- **Helium (He):** $1s^2$ (K shell)
- **Sodium (Na):** $1s^2 2s^2 2p^6 3s^1$ (K, L, and M shells)

Distribution of Electrons in Subshells

Following rules are applied to fill the orbitals of multi-electron atoms.

Aufbau Principle

Aufbau principle is also known as the building up principle. This principle says ***that the subshells in an atom are filled with electrons in an increasing order of their energy values.***

Arrangement of the subshells energy wise:

The energy of a subshell in the absence of any magnetic field, depends upon the principal quantum number (n) and the azimuthal quantum number (l).

Thus the order of filling subshells with electrons may be obtained from the summation $(n + l)$. $(n + l)$ values are given in Table.

Table: $(n + l)$ values of various sub-shells.

Principal quantum no. (n)	Azimuthal quantum no. (l)	Subshell	$(n+l)$ Value
1	0	1s	$(1 + 0) = 1$
2	0 1	2s 2p	$(2 + 0) = 2$ $(2 + 1) = 3$
3	0 1 2	3s 3p 3d	$(3 + 0) = 3$ $(3 + 1) = 4$ $(3 + 2) = 5$
4	0 1 2 3	4s 4p 4d 4f	$(4 + 0) = 4$ $(4 + 1) = 5$ $(4 + 2) = 6$ $(4 + 3) = 7$

a) The subshell having lower $(n + l)$ value has lower energy and is filled first.

For example, 4 s orbital has $(n + l) = 4 + 0 = 4$ and 3d orbital has $(n + l) = 3 + 2 = 5$. Since $(n + l)$ value of 4s orbital is lower than that of 3d, hence 4 s subshell has lower energy than 3d and 4s will be filled first.

b) In case there are two subshells are having equal $(n + l)$ values, then the subshell with lower 'n' value will be filled first.

For example, both 4p and 3d subshells have n + 1 value equal to 5(4p = 4 + 1 = 5) and (3d = 3 + 2 = 5); 3d subshell will be preferred to be filled because of its low n value.

According to this rule the energy wise arrangement of orbitals should be.

1s < 2s < 2p < 3 s < 3p < 4 s < 3d < 4p < 5 < 4 d < 5 < s < 4f < 5d < 6 < 7 s

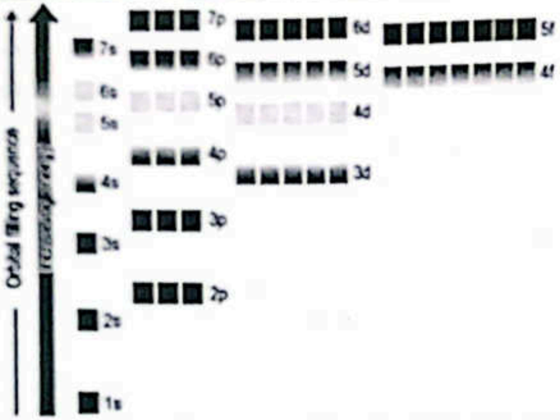


Fig: The diagram shows the energy of each subshell. Each box on the diagram represents an atomic orbital.

So, the order of filling of various subshells with electrons obtained by this rule is given below Figure.

Pauli's Exclusion Principle

According to this principle:

"No two electrons in an atom can have the same values for all the four quantum numbers"

Or

"Two electrons in an orbital will always have opposite spins".

Explanation:

In the first shell of helium (He) atom, there are two electrons. They are present in 1 s orbital. According to the concept of quantum numbers and Pauli's exclusion principal, the values of their quantum numbers are:

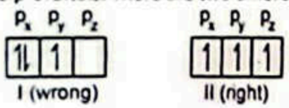
Table values of quantum numbers of two electrons in the same orbital

Electron	n	l	m	s
Electron 1	1	0	0	$+\frac{1}{2}$ (clockwise)
Electron 2	1	0	0	$-\frac{1}{2}$ (anticlockwise)

The two electrons having the same values of 'n', 'l' and 'm' can have different values of 's'. It means that their spins are in the opposite directions.

Hund's Rule

This rule gives an idea for filling electrons into the orbitals having equal energies. For example, three p-orbtials, i.e., p_x, p_y and p_z have equal energy. To understand it, let us take an example in which three electrons are to be filled into three p-orbitals. There are two different ways to do this as shown below:



The structure II is correct. Hund's rule, states that,

When degenerate orbitals are available and more than two electrons are to be placed in them, they should be placed in separate orbitals with the same spin rather than in the same orbital with opposite spins.

- According to the Hund's rule, the correct way of filling three electrons in three p orbitals is that in which each orbital is singly occupied.

Filling the Orbitals

A useful way of representing electronic configurations is a diagram that places electrons in boxes Figure.

- Each box represents an atomic orbital.
- The boxes (orbitals) can be arranged in order of increasing energy from bottom to top.

- An electron is represented by an arrow.
- The direction of the arrow represents the 'spin' of the electron.
- When there are two electrons in an orbital, the 'spins' of the electrons are opposite, so the two arrows in this box point in opposite direction.
- Electrons in the same region of space repel each other because they have the same charge.
- So wherever possible, electrons will occupy separate orbitals in the same subshell to minimize this repulsion. These electrons have the same 'spins' in different orbitals.
- Electrons are only paired when there are no more empty orbitals available within a subshell.

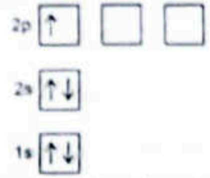


Figure: The electronic configuration of boron

Figure: shows the electronic structures of carbon, nitrogen and oxygen to illustrate these points

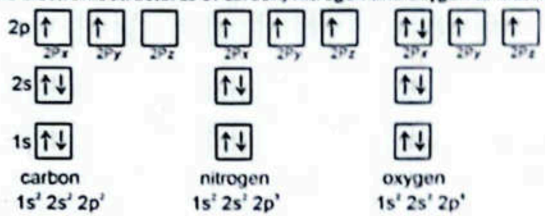


Figure: When adding electrons to a particular subshell, the electrons are only paired when no more empty orbitals are available.

The electron configurations of some elements of the periodic table in the light of the abovementioned principles are given in Table.

Table: Electronic configuration of ground states of elements Z = 1–36.

Z	Element	Configuration	Z	Element	Configuration
1.	H	$1s^1$	19.	K	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^1$
2.	He	$1s^2$	20.	Ca	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2$
3.	Li	$1s^2 2s^1$	21.	Sc	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^1 4s^2$
4.	Be	$1s^2 2s^2$	22.	Ti	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^2 4s^2$
5.	B	$1s^2 2s^2 2p^1$	23.	V	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^3 4s^2$
6.	C	$1s^2 2s^2 2p^2$	24.	Cr	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^5 4s^1$
7.	N	$1s^2 2s^2 2p^3$	25.	Mn	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^5 4s^2$
8.	O	$1s^2 2s^2 2p^4$	26.	Fe	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^6 4s^2$
9.	F	$1s^2 2s^2 2p^5$	27.	Co	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^7 4s^2$
10.	Ne	$1s^2 2s^2 2p^6$	28.	Ni	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^8 4s^2$
11.	Na	$1s^2 2s^2 2p^6 3s^1$	29.	Cu	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^1$
12.	Mg	$1s^2 2s^2 2p^6 3s^2$	30.	Zn	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2$
13.	Al	$1s^2 2s^2 2p^6 3s^2 3p^1$	31.	Ga	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^1$
14.	Si	$1s^2 2s^2 2p^6 3s^2 3p^2$	32.	Ge	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^2$
15.	P	$1s^2 2s^2 2p^6 3s^2 3p^3$	33.	As	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^3$
16.	S	$1s^2 2s^2 2p^6 3s^2 3p^4$	34.	Se	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^4$
17.	Cl	$1s^2 2s^2 2p^6 3s^2 3p^5$	35.	Br	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^5$
18.	Ar	$1s^2 2s^2 2p^6 3s^2 3p^6$	36.	Kr	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6$

ELECTRONIC CONFIGURATION AND THE PERIODIC TABLE

- We have seen that the electron configurations of elements are related to their position in the periodic table. The periodic table is structured so that elements with the same pattern of outer-shell (valence) electron configuration are arranged in same groups.
- We can easily write the electron configuration of an element based on its location in the periodic table. The pattern is summarized in Figure. Notice that the elements can be grouped in terms of the type of orbital into which the electrons are placed.
- ***On the left are two columns of elements. These elements, known as the alkali metals and alkaline earth metals (groups 1 and 2), are those in which the outer-shell s orbitals are being filled.***
- We see that the group 1 and 2 elements all have ns^1 and ns^2 outer configurations respectively.
- When we jump to group 13 elements, we find that they have ns^2np^1 configuration.
- ***On the right is a block of six columns. These are the elements in which the outermost 'p' orbitals are being filled.***
- ***In the middle of the table is a block of ten columns that contain the transition metals. In these, the d orbitals are being filled.***
- Below the main portion of the table are two rows that contain fourteen columns. These elements are often referred to as the f-block elements. These are the ones in which the 'f' orbitals are being filled. Recall that the numbers 2, 6, 10, and 14 are precisely the number of electrons that can fill the s, p, d, and f subshells, respectively.

> **Rack Your Brain!**
> 9. Write electronic configuration of Cu_{29} and I_{53}.

> **Rack Your Brain!**
> 10. Distribute electrons in the orbitals of: (A) Ca_{20} (B) Cs_{55}

QUICK CHECK 2.5

a) With the help of periodic table, write the electronic configurations for the following elements by giving the appropriate noble-gas inner core plus the electrons beyond it (i) $_{48}Cd$; (ii) $_{57}La$.

Ans. (i) $_{48}Cd$ = $1s^2, 2s^2, 2p^6, 3s^2, 3p^6, 4s^2, 3d^{10}, 4p^6, 5s^2, 4d^{10}$
= $[Kr]4d^{10}5s^2$

(ii) $_{57}La$ = $1s^2, 2s^2, 2p^6, 3s^2, 3p^6, 4s^2, 3d^{10}, 4p^6, 5s^2, 4d^{10}, 5p^6, 6s^2, 5d^1$
= $[Xe]5d^16s^2$

b) Write the complete electron configuration for antimony (Sb) with atomic number 51.

Ans. $_{51}Sb$ = $1s^2, 2s^2, 2p^6, 3s^2, 3p^6, 4s^2, 3d^{10}, 4p^6, 4d^{10}, 5s^2, 5p^3$
= $[Kr]4d^{10}5s^25p^3$

c) How many unpaired electrons are there in each atom of $_{51}Sb$?

Ans. Number of unpaired electrons in $_{51}Sb$ = 03 (three)
$5px^1, 5py^1, 5pz^1$

d) Write down the electronic configuration of valence shell of the following in terms of orbitals:
i) $_{13}Al$ ii) $_{14}Si$ $_{28}Ni$

Ans. The valence shell electronic configurations in terms of orbitals for the given elements:
i) Aluminium ($_{13}Al$): $3s^2\ 3p^1$ ii) Silicon ($_{14}Si$): $3s^2\ 3p^2$ iii) Nickel ($_{28}Ni$): $3d^8\ 4s^2$

Valence Electrons

The electrons in an atom in the outermost shell are called valence electrons. These are such electrons that are primarily involved in chemical reactions.

The similarities among the configurations of valence electrons account for similarities of the chemical properties among groups of elements.

Figure shows a periodic table which include the valence shell configurations included. Note the similarity in electron configuration within any group (column) of elements.

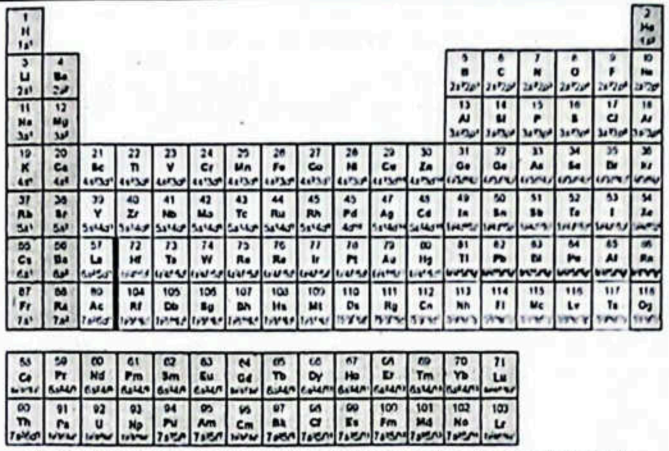


Figure: The electronic distribution of elements of modern periodic table

Classification of Elements of Periodic Table

The main-group or representative elements all have valence-shell configurations ns^anp^b. They have some choice of 'a' and 'b'. In other words, the outer 's' or 'p' subshell is being filled. Similarly, in the d-block transition elements, a 'd' subshell is being filled. In the *f*-block transition elements or inner-transition elements, an '*f*' subshell is being filled.

There is a definite pattern to the order of filling of the subshells as we go through the elements in the periodic table. From this we can write down the building-up order. The overall sketch of periodic table is given in Figure. This shows the blocks of elements.

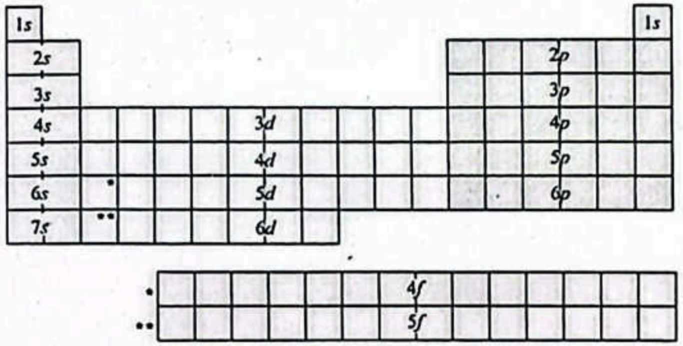


Figure: Modern periodic table showing s, p, d and f-block elements.

Figure shows a periodic table indicating this pattern. For example, in the blue colored area, an 'ns' subshell is being filled. In the green colored area, an np subshell is being filled. In the yellow area, an (n – 1)d subshell is being filled. In the light golden area and (n – 2)*f* subshell is being filled.

We start building-up order by starting with the first period, in which the '1s' subshell is being filled. In the second period, we have '2s'; then staying in the same period but jumping across, we have '2p'. In the third period, we have '3s' and '3p'; in the fourth period, '4s', '3d' and then '4p'. This pattern should become clear enough to visualize with a periodic table.

- The classification of elements of periodic table has been done into metals, non-metals, representative, transition elements, periods, groups and blocks (s, p, d, f). This division is done on the basis of electronic configuration and their valence electrons. The chemical properties of various categories of elements discussed above can be easily assessed.

QUICK CHECK 2.6

a) An element has the electronic configuration: $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6 4d^{10} 5s^2 5p^5$

i. Which block in the Periodic Table does this element belong to?
Ans. p-block
ii. Which group does it belong to?
Ans. Halogens
iii. Which period does it belong to?
Ans. 5
iv. Identify this element.
Ans. Iodine

b) Which block in the periodic table does the element with the electronic configuration $1s^2 2s^2 2p^6 3s^2 3p^6 3d^5 4s^1$ belong to? Name it.
Ans. d-block and the element is Chromium (Cr).

ELECTRONIC CONFIGURATION OF IONS AND FREE RADICALS

Ions

Positive Ions: ***Positive ions are formed when electrons are removed from atoms.***

The sodium ion, Na^+ (proton number = 11), has 10 electrons. So, its electronic configuration is $1s^2 2s^2 2p^6$
Note that this is the same as the electronic configuration of neon, the element with 10 electrons in each atom.

Negative Ions: ***Negative ions are formed when atoms gain electrons.***

The sulfide ion, S^{2-} (proton number = 16), has 18 electrons. Its electronic configuration $1s^2 2s^2 2p^6 3s^2 3p^6$, which is the same as argon, the element with 18 electrons in each atom.

Note that, in general, electrons in the outer subshell are removed when metal atoms form the positi ions. However, the d-block elements behave slightly differently. Reading across the Periodic Table fro potassium to zinc, the 4 s subshell fills before the 3 d subshell. But when atoms of a d-block element lo electrons to form ions, the 4 s electrons are lost first.

For example:

- Ti atom: $1s^2 2s^2 2p^6 3s^2 3p^6 3d^2 4s^2$
- Ti^{2+} ion: $1s^2 2s^2 2p^6 3s^2 3p^6 3d^2$
- Cr atom: $1s^2 2s^2 2p^6 3s^2 3p^6 3d^5 4s^1$
- Cr^{3+} ion: $1s^2 2s^2 2p^6 3s^2 3p^6 3d^3$

Free Radicals

"A free radical is a species that has one or more unpaired electrons".
For example: Free chlorine atom:

$Cl^\bullet$: The electron configuration of this radical is $1s^2 2s^2 2p^6 3s^2 3p^5$. In the 2p subshell, two orbitals ha paired electrons whereas, the third one contains a single unpaired electron. The unpaired electron shown by a single dot as in $Cl^\bullet$. Apart from single atoms, groups of atoms can also be free radicals. F example, $OH^\bullet$, $CH_3^\bullet$, etc.

QUICK CHECK 2.7

Write electronic configurations for the following ions and free radicals:

i. $Al (Z=13)$
Ans. $1s^2, 2s^2, 2p^6, 3s^2, 3p^1$

ii. $O^{2-} (Z=8)$
Ans. $1s^2, 2s^2, 2p^6$

iii. $Fe^{3+} (Z=26)$
Ans. $1s^2, 2s^2, 2p^6, 3s^2, 2p^6, 3d^5$

iv. $Cu^{2+} (Z=29)$
Ans. $1s^2, 2s^2, 2p^6, 3s^2, 3p^6, 3d^9$

v. $Cu (Z=29)$
Ans. $1s^2, 2s^2, 2p^6, 3s^2, 3p^6, 3d^{10}, 4s^1$

ELECTRONIC CONFIGURATION AND THE FORMATION OF SEMICONDUCTORS

Semi-Conductors

"The materials whose electrical conductivity lies in between that of conductors and insulators are called semiconductors".

According to number of elements, these are classification into two classes:
(i) Elemental Semiconductors **(ii) Compound Semiconductors**

Semiconductors are materials that can conduct electricity under some conditions. They are used in many electronic devices, including smartphones, laptops, and cars.

Examples: Silicon, germanium and arsenic etc. The formation of semiconductors is possible because of a unique electronic configuration of these elements.

Silicon as Semiconductor:

Consider the example of Si and explore how it can be converted into a p-type and n-type semiconductors.

The electron configuration of $_{14}Si = 2,8,4$; meaning that it has 4 electrons in its valence shell. In the pure crystalline form, each Si atom is bonded to four other Si atoms. In this form, there is no possibility of electronic conduction through the Si crystal.

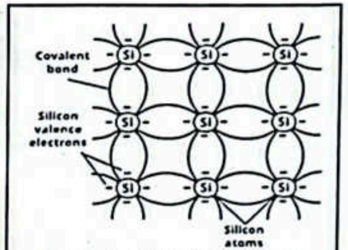


Figure: A crystal of pure silicon

P-type and N-type semiconductors are formed by "doping" a pure semiconductor material with impurity atoms, where adding trivalent impurities (like boron or aluminum) creates a P-type semiconductor, while adding pentavalent impurities (like phosphorus or arsenic) creates an N-type semiconductor.

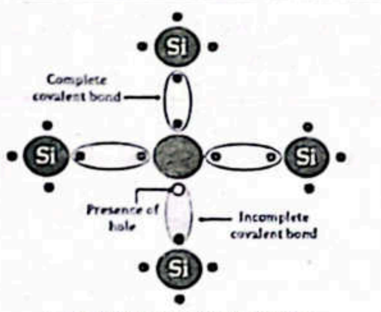
The difference lies in whether the added impurity creates "holes" (positive charge carriers) in the lattice, leading to P-type, or extra electrons (negative charge carriers) leading to N -type.

P-type Semiconductor Formation

- Impurity atoms with three valence electrons (like Al) are added to the pure semiconductor.
- Some of the trivalent atoms take place of the Si atoms in the crystals.
- The silicon atoms cannot make four bonds due to the lack of electrons.
- For this reason, there are created holes in the crystal lattice, which act as positive charge carriers as shown in Figure.
- This process creates a positive-type semiconductor or N-type semiconductor.
- Electrons from an external current source can move through the semiconductor and it can act as a conductor.

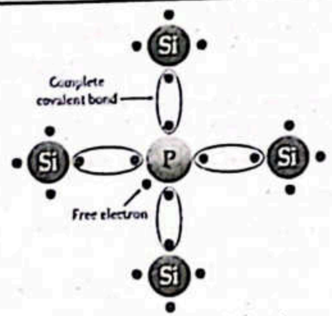
N-type Semiconductor Formation

- When impurity atoms with five valence electrons (like phosphorus) are added to the pure semiconductor, some of Si atoms are replaced with the pentavalent phosphorus atoms.
- The Si atoms in the vicinity of these atoms can make four bonds and the fifth electron is an extra electron.
- These impurity atoms contribute extra electrons to the crystal lattice, which become free to move and act as negative charge carriers as in Figure.
- The result is an N-type semiconductor that can conduct electricity when connected to an external source.



- Si = Intrinsic semiconductor atom
- Al = Trivalent impurity atom

Formation of P type extrinsic semiconductor



- Si = Intrinsic semiconductor atom
- P = Pentavalent impurity atom

Formation of N type extrinsic semiconductor

Figure: Doping and the formation of P-type and N-type semiconductor

Solution File — Rack Your Brain!

Sr. #	Option	Explanation
1.	D	P = 6, n = 8, e = 6, ⇒ total = 20 fundamental particles.
2.	S.Q	In the absence of any electric or magnetic field, cathode rays move in straight line perpendicular to the surface of cathode. In 1895, J. Perrin showed that when cathode rays are passed between the poles of the magnet, the cathode rays was deflected which showed that they have charge. In 1897, Sir J.J. Thomson established their electric charge by the application of electric field. The cathode rays deflected towards positive plate showing their negative nature.
3.	C	Quantum number values for '3d' orbital will be $n = 3$, $\ell = 2$
4.	D	Quantum number value for 2s orbitals are $n = 2$, $\ell = 0$
5.	C	The value of $(n + \ell)$ for the 3d sub-shell = 3 + 2 = 5.
6.	B	The value of $(n + \ell)$ for the 5s sub-shell = 5 + 0 = 5.
7.	S.Q	For $\ell = 3$ as $\ell = 3$ and subshell is 'f'. This shows that f-subshell has 7 different ways of orientation in space because it has 7 values of magnetic quantum number When $\ell = 3$, then m = 0, ±1, ±2, ±3 = 7 values i. f_{x^3} ii. f_{y^3} iii. f_{z^3} iv. f_{xyz} v. $f_{x^2-y^2}$ vi. $f_{y^2-z^2}$ vii. $f_{x^2-z^2}$
8.	S.Q	The formula for calculating electrons is $2(2\ell + 1)$. When $\ell = 0$ s-subshell total electrons = 2 $\ell = 1$ p-subshell total electrons = 6 $\ell = 2$ d-subshell total electrons = 10 $\ell = 3$ f-subshell total electrons = 14
9.	S.Q	Element — Electronic Configuration Copper 29(Cu) — $1s^2 2s^2 2p^6 3s^2 3p^6 4s^1 3d^{10}$ Iodine 53(I) — $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^2 4d^{10} 5p^5$
10.	S.Q	Element — Electronic Configuration Calcium 20(Ca) — $1s^2 2s^2 2p^6 3p^2 3p^6 4s^2$ Cesium 55(Cs) — $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 4d^{10} 5s^2 5p^6 6s^1$

Exercise

MULTIPLE CHOICE QUESTIONS (MCQs)

Q.1 Four choices are given for each question. Select the correct choice.

I. The quantum number ' m ' of a free gaseous atom is associated with:
a) the effective volume of the orbital
b) the shape of the orbital
c) the spatial orientation of the orbital
d) the energy of the orbital in the absence of a magnetic field

II. When 3d subshell is completely filled, the next entering electron goes into:
a) 4f b) 4s c) 4p d) 4d

III. Quantum number values for 2p orbitals are:
a) $n=2, \ell=1$ b) $n=1, \ell=2$ c) $n=1, \ell=0$ d) $n=2, \ell=0$

IV. An electron having the set of values: $n=4, \ell=0, m=0$ and $s=+1/2$ lies in:
a) 2s b) 3s c) 4s d) 5s

V. The quantum number values for the fourth electron of $^{9}_{4}Be$ atom are:
a) 1, 0, 0 b) 2, 0, 0 c) 2, 1, 0 d) 1, 1, 1

VI. The correct order of first ionization energies is:
a) F>He>Mg>N>O b) He>F>N>O>Mg c) He>O>F>N>Mg d) N>F>He>O>Mg

VII. A p orbital has a characteristic shape with how many lobes?
a) 1 b) 2 c) 3 d) 4

VIII. The three p orbitals in a given energy level are oriented:
a) Along the same axis.
b) At 45° to each other.
c) Mutually perpendicular to each other along the x, y, and z axes.
d) In a complex tetrahedral arrangement.

IX. How many d orbitals are there in a given energy level?
a) 1 b) 3 c) 5 d) 7

X. What information does the principal quantum number (n) give us about orbitals?
a) Size b) Shape c) Size and shape d) Spin

XI. How many unpaired electrons are present in an atom of cobalt?
a) Two b) Three c) Four d) Five

Answer Key with Explanations

Sr.No.	Option	Answer	Explanation
I.	c	the spatial orientation of the orbital	• The magnetic quantum number (m) determines the orientation of an orbital in space (e.g., p_x, p_y, p_z).
II.	c	4p	• After filling 3d, the next electron enters 4p (Aufbau order: 3d → 4p).
III.	a	$n = 2$, $\ell = 1$	• For 2p orbitals: o Principal quantum number (n) = 2. o Azimuthal quantum number (ℓ) = 1 (for p-subshell).
IV.	c	4s	• Quantum numbers n=4, ℓ=0 indicate a 4s orbital (ℓ=0 for s-orbitals).

V.	b	2, 0, 0	• Beryllium (Be, Z = 4): Electron configuration = $1s^2 2s^2$. • The 4th electron is in 2s: n=2, l=0, m=0.
VI.	b	He > F > N > O > Mg	• Ionization energy trend: Noble gases (He) > halogens (F) > N > O > metals (Mg). • N > O due to half-filled 2p subshell stability.
VII.	b	2	• A p orbital has two lobes (dumbbell shape) with a nodal plane at the nucleus.
VIII.	c	Mutually perpendicular to each other along the x, y, and z axes	• The three p orbitals (p_x, p_y, p_z) are oriented 90° apart along Cartesian axes.
IX.	c	5	• Each energy level has 5d orbitals (dxy, dxz, dyz, dx^2-y^2, dz^2).
X.	a	Size	The principal quantum number (n) determines the size of an orbital. As the value of n increases, the size of the orbital also increases. The principal quantum number (n) does not determine the shape of an orbital; that's determined by the azimuthal quantum number (l). Spin of orbital is determined by Magnetic quantum number.
XI.	b	Three	Cobalt's atomic number is 27. Its electronic configuration is [Ar] $3d^7 4s^2$. According to Hund's rule, the 3d electrons occupy the orbitals with maximum spin multiplicity, resulting in 3 unpaired electrons.

SHORT ANSWER QUESTIONS

Q.2 Attempt the following short-answer questions:

a. There are three orientations of p-orbital due to three values of magnetic quantum number. Justify it.

Ans. It is correct. There are three orientations of the p-orbital due to the three values of the magnetic quantum number (m_l). Here's the justification in simple scientific terms:

Quantum Numbers:

Each electron in an atom is described by four quantum numbers:

1. Principal quantum number (n) – energy level
2. Azimuthal/angular quantum number (l) – shape of orbital
3. Magnetic quantum number (m_l) – orientation of orbital
4. Spin quantum number (m_s) – spin direction of electron

For a p-orbital:

- The azimuthal quantum number (l) = 1
- (Because p-orbitals correspond to l = 1)
- The magnetic quantum number (m_l) can have three values:

$$m l = -1, 0, +1 m l = -1, 0, +1 m l = -1, 0, +1$$

b. 'I_3' of Mg is much bigger than its 'I_2'. Justify.

Ans. The third ionization energy (I_3) of magnesium (Mg) is much bigger than its second ionization energy (I_2). Here's the scientific justification:

- Ionization energy is the energy needed to remove one electron from an atom or ion.
- I_1: Remove 1st electron
- I_2: Remove 2nd electron
- I_3: Remove 3rd electron

Electronic Configuration of Magnesium:

Neutral Mg atom:

Mg (Z = 12) = $1s^2 2s^2 2p^6 3s^2$

- First ionization (I_1) removes one electron from $3s^2$ → becomes Mg^+
- Second ionization (I_2) removes second 3s electron → becomes Mg^{2+}
- Third ionization (I_3) would now try to remove an electron from the $2p^6$ (inner, noble gas core)

After removing two outermost 3s electrons, Mg^{2+} has the stable configuration of Neon (Ne):

$$Mg^{2+} = 1s^2 2s^2 2p^6$$

Now, the third electron to be removed is from a completely filled inner shell (2p), which:

- Is very stable (noble gas configuration)
- Is closer to the nucleus
- Is more strongly attracted by nuclear charge

Hence, much more energy is needed to remove this tightly bound electron.

c. Among the elements Li, K, Ca, S and Kr which one has the lowest first ionization energy? Which has the highest first ionization.

Ans. Ionization Energy Trend Recap:

- Increases across a period (left → right) due to increasing nuclear charge.
- Decreases down a group (top → bottom) as outer electrons are farther from the nucleus and more shielded.

Element	Group	Period	Electron Configuration	Notes
Li (Lithium)	1	2	$1s^2 2s^1$	Alkali metal (low IE)
K (Potassium)	1	4	[Ar] $4s^1$	Lower IE than Li (further down)
Ca (Calcium)	2	4	[Ar] $4s^2$	Slightly higher IE than K
S (Sulphur)	16	3	[Ne] $3s^2 3p^4$	Nonmetal (higher IE)
Kr (Krypton)	18	4	[Ar] $3d^{10} 4s^2 4p^6$	Noble gas (very high IE)

- Lowest first ionization energy = Potassium (K)
- Reason: It's a Group 1 element in Period 4 → outermost electron is loosely held and easily removed.
- Highest first ionization energy = Krypton (Kr)
- Reason: Noble gas with a full outer shell → very stable → requires lots of energy to remove an electron.

d. Consider the electronic configuration of the potassium atom (atomic number 19).

Ans. Element: Potassium (K)

Atomic Number: 19

So it has 19 electrons.

Electronic Configuration:

$1s^2 2s^2 2p^6 3s^2 3p^6 4s^1$

(i) Write the full electronic configuration of potassium using the s, p, d, f notation.

Ans. Element: Potassium (K)

Atomic Number: 19

So it has 19 electrons.

Electronic Configuration:

$1s^2 2s^2 2p^6 3s^2 3p^6 4s^1$

(ii) Explain why the 4s subshell is filled before the 3d subshell in potassium, even though the principal quantum number of the 3d subshell is lower.

Ans. Even though:

- 3d has a lower principal quantum number (n = 3)
- 4s has a higher principal quantum number (n = 4)

The 4s subshell has *lower energy* than 3d at the time potassium's electrons are being placed.

Key Principles:

1. **Aufbau Principle**
   Electrons fill orbitals in order of increasing energy, not just by n value. According to the Aufbau (building-up) principle:

   $$1s < 2s < 2p < 3s < 3p < 4s < 3d < 4p$$

   As you can see, **4s comes before 3d.**
2. **Energy Level Overlap**
   - 4s orbital is farther from the nucleus but has less electron-electron repulsion, making it lower in energy than 3d.
   - So, the first 19 electrons (in potassium) go into the 4s before starting to fill 3d.

Potassium (Z = 19):

- **Configuration:** $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^1$
- The 3d subshell remains empty in potassium because it's higher in energy at this point.

Conclusion:

The 4s subshell is filled before 3d in potassium because, despite having a higher principal quantum number, it is lower in energy at the point when electrons are added, following the Aufbau principle.

e.(i) An atom of element X has an atomic number of 17 and a mass number of 35. Determine the number of protons, neutrons, and electrons in this atom.

Ans. Number of Protons = Atomic Number
Protons = 17
Number of Neutrons = Mass Number – Atomic Number
Neutrons = 18
Number of Electrons = Number of Protons (in a neutral atom)
Electrons = 17

(ii) If this element forms an ion with a charge of –1, how many protons, neutrons, and electrons will be present in the ion?

Ans. X element has:

- Atomic number = 17
- Mass number = 35

We previously identified it as chlorine (Cl).
Now, let's consider the Cl^- ion (chloride ion), which has a -1 charge.

Protons

- The number of protons never changes, even when forming ions.

Protons = 17

Neutrons

- Mass number = 35, Atomic number = 17

Neutrons = 18

Electrons (for Cl^- ion)

- Neutral chlorine atom has 17 electrons
- A –1 charge means it has gained one extra electron

Electrons = 17+1 = 18

f. In the ground state of mercury $_{80}Hg$:

Ans. In the ground state of mercury (Hg), which has an atomic number of 80, we can determine several important features of the atom, such as its **electron configuration**, and the number of **protons, neutrons** and electrons.

Basic Information for Mercury (Hg):

- **Symbol:** Hg
- **Atomic number (Z):** 80 → Protons = 80, Electrons = 80 (in a neutral atom)
- **Mass number (most common isotope):** 200 → So, Neutrons = 200 – 80 = 120

Ground-State Electron Configuration:

Mercury is a transition metal, and its full electron configuration is:

$$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^6\ 5s^2\ 4d^{10}\ 5p^6\ 6s^2\ 4f^{14}\ 5d^{10}$$

In noble gas short hand:

$$[Xe]\ 4f^{14}\ 5d^{10}\ 6s^2$$

i. How many electrons occupy atomic orbitals with n = 3?

Ans. Electrons can occupy atomic orbitals where the principal quantum number n = 3n = 3n = 3.
For n = 3n = 3n = 3, the possible subshells (values of ℓ) are:

- ℓ = 0\ell = 0 ℓ=0 → 3s
- ℓ = 1\ell = 1 ℓ=1 → 3p
- ℓ = 2\ell = 2 ℓ=2 → 3d

Each subshell has a certain number of orbitals, and each orbital holds 2 electrons:

Subshell	Orbitals	Electrons
3s	1	2
3p	3	6
3d	5	10

Total electrons when n = 3n = 3n = 3:

2 (3s) + 6 (3p) + 10 (3d) = 18 electrons

So, 18 electrons can occupy atomic orbitals with principal quantum number n = 3n = 3n = 3.

ii. How many electrons occupy 4d atomic orbitals?

Ans. The 4d atomic orbitals can hold a maximum of 10 electrons. This is because the 4d subshell consists of 5 orbitals (each orbital can hold a maximum of 2 electrons), so 5 orbitals × 2 electrons = 10 electrons in total.

iii. How many electrons occupy $4p_z$ atomic orbital?

Ans. The 4pz atomic orbital can hold a maximum of 2 electrons. Each atomic orbital, including the 4pz orbital, can accommodate up to 2 electrons, with each electron having opposite spins.

iv. How many electrons in the valence shell have spin "up" ($s = -\frac{1}{2}$)?

Ans. In an atomic orbital, each electron can have one of two possible spins: "up" (denoted as $s = +\frac{1}{2}$) or "down" (denoted as $s = -\frac{1}{2}$).

If you are asking how many electrons have a spin of $s = -\frac{1}{2}$ in a particular orbital, it depends on how many electrons are present in that orbital. For example:

- In a single atomic orbital (such as the 4pz orbital), a maximum of 2 electrons can occupy it, one with spin $+\frac{1}{2}$ and one with spin $-\frac{1}{2}$.
- If there are multiple orbitals (such as in a subshell like the 4d or 4p), the electrons will fill the orbitals according to the Pauli exclusion principle, with one electron having spin $+\frac{1}{2}+\frac{1}{2}+\frac{1}{2}$ and the other having spin $-\frac{1}{2}$ in each orbital.

So, in general, half of the electrons in any set of orbitals would have spin $s = -\frac{1}{2}$, assuming the electrons are paired and fill orbitals according to Hund's rule and the Pauli exclusion principle.

Conclusion: 80 electrons in total and thus 40 orbitals in Hg.

g. The successive ionization energies for an unknown element are

$I_1 = 896\ kJ/mol$ $I_2 = 1752\ kJ/mol$

$I_3 = 14,807\ kJ/mol$ $I_4 = 17,948\ kJ/mol$

To which family in the periodic table, does the unknown element most likely belong?

Ans. As there is greatest difference between 2nd and 3rd ionization energies, it means this element belongs to group 2A (Alkaline Earth's metal).

i. Consider the following ionization energies for aluminum:

$Al_{(g)} \longrightarrow Al^{+}_{(g)} + e^-$ $I_1 = 580\ kJ/mol$

$Al^{+}_{(g)} \longrightarrow Al^{2+}_{(g)} + e^-$ $I_2 = 1815\ kJ/mol$

$Al^{2+}_{(g)} \longrightarrow Al^{3+}_{(g)} + e^-$ $I_3 = 2740\ kJ/mol$

$Al^{3+}_{(g)} \longrightarrow Al^{4+}_{(g)} + e^-$ $I_4 = 11,600\ kJ/mol$

(i) Account for the trend in the values of the ionization energies.

(ii) Explain the large increase between I_3 and I_4.

(iii) List the four aluminum ions given in order of increasing size, and explain your ordering.

Ans.

(i) $I_4 > I_3 > I_2 > I_1$

(ii) As there is greatest difference between 3rd and 4th ionization energies, it means this element belongs to group 3A (Boron family).

(iii) After loosing 3rd electron, Aluminium gets stable electronic configuration of noble gas.

$$\underset{2,8,3}{Al} \longrightarrow \underset{2,8}{Al^{3+}} + 3e^-$$

$$\underset{\substack{13p\\9e}}{Al^{4+}} < \underset{\substack{13p\\10e}}{Al^{3+}} < \underset{\substack{13p\\11e}}{Al^{2+}} < \underset{\substack{13p\\12e}}{Al^{1+}}$$

In Al^{+1} there are 13 protons and 12 electrons so, control of nucleus is lesser on outer electrons so its size is greatest among above.

In Al^{+4} there are 13 protons and 9 electrons, there is more imbalance between proton to electron ratio so, control of nucleus is greatest and its size is the least among above.

h. (i) State the general order of filling orbitals up to the 4p subshell.

(ii) Explain why the 4s subshell is filled before the 3d subshell, according to the Aufbau principle.

Ans. (i) $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^6$

(ii) The 4s subshell is filled before the 3d subshell according to the Aufbau principle because the 4s orbital is lower in energy than the 3d orbital when these orbitals are empty or partially filled in neutral atoms.

1. Energy Considerations:

- Even though 4s has a higher principal quantum number (n = 4) than 3d (n = 3), the energy of an orbital depends on both the principal quantum number n and the azimuthal quantum number ℓ.
- For 4s: n = 4, ℓ = 0, so n + 1 = 4
- For 3d: n = 3, ℓ = 2, so n + 1 = 5

- According to the (n + ℓ) rule (used in the Aufbau principle), orbitals with a lower n + ℓ value are filled first.

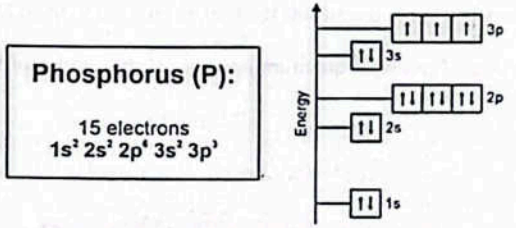
2. Electron Shielding and Penetration:

- The 4s orbital penetrates closer to the nucleus and experiences less shielding than the 3d orbital.
- As a result, electrons in the 4s orbital are more tightly held and thus occupy a lower energy level initially.

However, once electrons are added to the 3d subshell, the energy levels shift slightly. In ions of transition metals, for example, the 4s electrons are usually lost before the 3d electrons, because the 4s orbital becomes higher in energy after the 3d subshell is filled or partially filled.

i. Draw the orbital box diagram for the valence electrons of a phosphorus atom (atomic number 15), ensuring that your diagram adheres to Hund's rule and the Pauli Exclusion Principle.

Ans.



DESCRIPTIVE QUESTIONS

Q.3 What are quantum numbers? Describe briefly principal and spin quantum numbers.

Ans. See Page No. (36)

Q.4 Draw the shapes of s, p and d-orbitals. Justify these by keeping in view the azimuthal and magnetic quantum numbers.

Ans. See Page No. (36)

Q.5 What do you mean by successive ionization energies? How the electronic shell structure of magnesium (Mg) is derived from the successive ionization energies?

Ans. See Page No. (33)

ADDITIONAL SLOs BASED MCQs

1. What does the electron configuration $1S^2 2S^2 2P^6$ represent?
   A. Carbon (C) B. Oxygen (O) C. Neon (Ne) D. Helium (He)
2. Which subshell can hold a maximum of 10 electrons?
   A. s B. p C. d D. f
3. How many unpaired electrons are there in the electron configuration d^5?
   A. 0 B. 1 C. 2 D. 5
4. Which element has the electron configuration $s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^8$?
   A. Iron (Fe) B. Zinc (Zn) C. Nickel (Ni) D. Copper (Cu)
5. What is the electron configuration of a chlorine ion (Cl^-)?
   A. $1s^2 2s^2 2p^6 3s^2 3p^6$ B. $1s^2 2s^2 2p^6 3s^2 3p^5$ C. $1s^2 2s^2 2p^6 3s^2 3p^7$ D. $1s^2 2s^2 2p^6 3s^2 3p^8$
6. As we move away from nucleus the distance between the adjacent orbits goes on:
   A. Increasing B. Decreasing
   C. Remains same D. May increase or decrease

7. Which of the following has the same number of electrons as that of α-particles:
A. Li^+ B. H^+ C. He^+ D. Be^{+2}

8. Which of the following orders with respect to relative energy is incorrect:
A. 2s < 2p B. 2p < 3p C. 3p < 3d D. 4d < 3s

9. After filling the 4s orbital the entering electron goes into:
A. 4p B. 5s C. 3d D. 4f

10. Which of the following particles contains 20 neutrons, 19 protons and 18-electrons?
A. ${}^{39}_{19}K^+$ B. ${}^{39}_{19}K$ C. ${}^{40}_{18}Ar$ D. ${}^{39}_{20}Ca$

11. Which of the following has maximum number of unpaired electrons?
A. Fe^{+3} B. Zn^{+2} C. Ni^{+2} D. Cu^+

12. According to (n + l) rule. Which one of the following has the highest energy?
A. 2s B. 3s C. 3p D. 2p

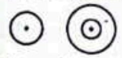
13. How many unpaired electrons are in the 3d sub-shells of an element with an Z = 24?
A. 2 B. 3 C. 4 D. 5

14. With increase in the value of principal quantum number 'n' the shapes of the s-orbital remain same although their sizes.
A. Increase B. Decrease
C. Remain the same D. May or may remain the same

15. The correct order of sub-shells, within a shell w.r.t decreasing energy is:
A. f > d > s > p B. f > d > p > s C. s > p > d > f D. p > s > f > d

Answer Key with Explanations

No.	Option	Explanations
1.	C	The electronic configuration of Ne = $1s^2 2s^2 2p^6$. It corresponds to a total of 10 electrons. Neon (Ne) is a noble gas.
2.	C	The d subshell can hold a maximum of 10 electrons, as it has five orbitals, with each orbital capable of holding two electrons.
3.	D	The electron configuration $3d^5$ indicates five electrons in the d subshell. According to Hund's rule, each of these five electrons will occupy a separate orbital in the d subshell, resulting in five unpaired electrons.
4.	C	The electron configuration $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^8$ corresponds to Nickel (Ni). The total 28 number of electrons, which shows the atomic number of Nickel.
5.	A	A chlorine ion (Cl^-) has gained one extra electron compared to the neutral chlorine atom, resulting in a full p orbital. The electron configuration of Cl^- thus becomes $1s^2 2s^2 2p^6 3s^2 3p^6$.
6.	A	Distance between shells can be calculated by $0.529n^2 A^\circ ; r_1 = 0.529 A^\circ$. So distance between consecutive shells is increasing continuously. $r_2 = 2.11 A^\circ$ $r_3 = 4.761 A^\circ$ $r_4 = 8.4 A^\circ$ $r_2 - r_1 < r_3 - r_2 < r_4 - r_3$
7.	B	α-particle similar to H^+ also have no electron's.
8.	D	According to $n + \ell$ rule 4d < 3s 4 + 2 < 3 + 0 6 < 3 Incorrect order
9.	C	According to $n + \ell$ rule after $4s \Rightarrow 4 + 0 = 4$ Entering $\bar{e}$ goes into $3d \Rightarrow 3 + 2 = 5$
10.	A	Among the following Potassium contain 20 neutrons, 19 protons and 18-electrons.

11.	A	$Fe^{+3} = 1s^2, 2s^2, 2P^6, 3s^2, 3P^6, 3d^5, 4s^0$ i.e., 5 unpaired electrons in 3d $Ni^{+2} = 1s^2, 2s^2, 2P^6, 3s^2, 3P^6, 3d^8, 4s^0$ i.e., 2 unpaired electrons in 3d $Cu^{+1} = 1s^2, 2s^2, 2P^6, 3s^2, 3P^6, 3d^{10}, 4s^0$ i.e., no unpaired electrons in 3d $Zn^{+2} = 1s^2, 2s^2, 2P^6, 3s^2, 3P^6, 3d^{10}, 4s^0$ i.e., no unpaired electrons in 3d
12.	C	2s = 2 + 0 = 2 3s = 3 + 0 = 3 3p = 3 + 1 = 4 2p = 2 + 1 = 3 Highest $(n + \ell)$ value is for 3P
13.	D	Z = 24 is Cr, $Cr_{24} = 1s^2, 2s^2, 2P^6, 3s^2, 3P^6, 3d^5, 4s^1$
14.	A	With the increase n value (principal quantum number), the size of s-orbital increases where as the shape remains the same. e.g. the size of 2s-orbital is greater than 1s-orbital.  1s 2s
15.	B	The correct order of sub-shells, within a shell w.r.t decreasing energy is f > d > p > s.

ADDITIONAL SHORT ANSWER QUESTIONS

Q.1 According to Moseley, the atomic number Z was a fundamental property of an element. How?

Ans. In 1913, Moseley v observed that when different elements were bombarded with cathode rays, the X-rays of some characteristic frequencies were produced. It was found that the square root of the frequency of the X-rays was directly proportional to the atomic number of an element Z.

$\sqrt{\text{frequency}}$ (v) α Z

He concluded that this number, i.e. the atomic number Z was a fundamental property of an element.

Q.2 What is effect of electric field on the fundamental particles?

Ans. The behaviour of particles in an electric field depends upon their mass and charge. They show their behaviour as follows.

- Neutrons being neutral are not deflected but travel in a straight path perpendicular to the direction of electric field.
- Protons being positively charged are deflected towards the negative plate.
- Electrons being negatively charged are deflected towards the positive plate.

Q.3 Differentiate between atomic spectra and atomic absorption spectrum.

Ans.

Atomic emission spectrum	Atomic absorption spectrum
When an element in its gaseous state is heated to high temperatures or subjected to electrical discharge, radiation of certain wavelengths is emitted. The spectrum of this radiation contains coloured lines and is called atomic emission spectrum.	When a beam of white light is passed through a gaseous sample of an element in cold state, certain wavelengths are absorbed. The wavelengths of the white light that has been absorbed by the atoms show up as dark lines on the spectrum. The spectrum of this radiation is called an atomic absorption spectrum.

Q.4 What is the trend of ionization energy in the periodic table?

Ans.
- As we go down a particular group, ionization energies decrease. The larger the atom, the easier is to separate an electron from it. Actually, down the group, number of shells increases, hold of nucleus on the valence electrons decreases, hence removal of electrons becomes easier.

- The ionization energies generally increase on going across a period. It is due to the reason that across the period shell number remains same. As the proton number increases, electrons are added in the same shell. Therefore, nucleus attracts the valence electrons more strongly. As a result, ionization energy increases across the period.

Q.5 Differentiate between shell and subshell.

Ans.

Shell	Subshell
• The collection of orbitals with the same values of n is called an electron shell • It is denoted by n.	• The set of orbitals that have the same n and ℓ values is called a subshell. • They are denoted by s,p,d and f.

Q.6 Define electronic configuration and give example.

Ans. Electronic configuration is the distribution of electrons among available shells, subshells, or orbitals of an atom or ion.

Example: the electronic configuration beryllium is given below,

$_5B = 1s^2, 2s^2, 2px^1, 2py^0, 2pz^0$

Q.7 State Hund's rule and Puali's exclusion principle.

Ans. Hund's rule: When degenerate orbitals are available and more than two electrons are to be placed in them, they should be placed in separate orbitals with the same spin rather than in the same orbital with opposite spins.

Puali's exclusion principle: According to this principle. No two electrons in an atom can have the same values for all the four quantum numbers or, "Two electrons in an orbital will always have opposite spins".

Q.8 Write the classification of the periodic table on the basis of electronic configuration.

Ans. The classification of elements of periodic table has been done into metals, non-metals, representative, transition elements, periods, groups and blocks (s, p, d, f). This division is done on the basis of electronic configuration and their valence electrons. The chemical properties of various categories of elements discussed above can be easily assessed.

Q.9 Write the electronic configuration of ions with examples.

Ans. Positive ions are formed when electrons are removed from atoms. The sodium ion, Na^+ (proton number = 11), has 10 electrons. So, its electronic configuration is $1s^2 2s^2 2p^6$.

Negative ions are formed when atoms gain electrons. The sulfide ion, S^{2-} (proton number = 16), has 18 electrons. Its electronic configuration is $1s^2 2s^2 2p^6 3s^2 3p^6$, which is the same as argon, the element with 18 electrons in each atom.

Q.10 What is the trend of ionization energy in the periodic table?

Ans. "A free radical is a species that has one or more unpaired electrons".

An example of a simple free radical is free chlorine atom $\cdot\ddot{C}l:$. The electron configuration of this radical is $1s^2 2s^2 2p^6 3s^2 3p^5$. In the 2p subshell, two orbitals have paired electrons whereas, the third one contains a single unpaired electron. The unpaired electron is shown by a single dot as in Cl.

Q.11 What is the trend of ionization energy in the periodic table?

Ans.

Property	p-type Semiconductor	n-type Semiconductor
Doping Element	Trivalent (like, Boron, Aluminium).	Pentavalent (like, Phosphorus, Arsenic).
Charge Carriers	Holes	Electrons
Type of Conduction	Mainly due to holes.	Mainly due to electrons.
Electrons in Conduction Band	Few	Many
Effect of Doping	It creates more holes.	Increases free electrons
Example	Positive side of a diode (anode).	Negative side of a diode (cathode).

SELF-ASSESSMENT Chapter # 02

Total Mark: 30

Q.1 Encircle the correct option. **(1 × 6 = 6)**

(i) When 3d subshell is completely filled, the next entering electron goes into:
A. 4f B. 4s C. 4p D. 4d

(ii) What is the shape of a p-orbital?
A. Spherical B. Dumbbell C. Circular D. Vertical

(iii) Quantum number values for 2p orbitals are:
A. n = 2, ℓ = 1 B. n = 1, ℓ = 2 C. n = 1, ℓ = 0 D. n = 2, ℓ = 0

(iv) Which principle states that electrons fill the lowest energy orbitals first?
A. Pauli's exclusion principle B. Hund's rule
C. Aufbau principle D. Heisenberg principle

(v) Which of the following species has a zero bond order according to MOT?
A. H_2^{1+} B. He_2^{1+} C. He_2^{2+} D. He_2

(vi) The number of protons, electrons, and neutrons in Na^+ are:
A. 11p, 11e, 12n B. 11p, 10e, 12n C. 11p, 12e, 11n D. 10p, 11e, 12n

Q.2 Write short answers of the following questions. **(2 × 8 = 16)**

(i) Size of Mg is bigger than Al, but ionization energy of Mg is more than that of Al. Why?
(ii) Define atomic number and how is it related to proton number?
(iii) How does ionic radius change compared to atomic radius in metals and nonmetals?
(iv) Define principal quantum number and orbital.
(v) Write the electronic configuration of Mg (Z = 12) using sub-shell notation.
(vi) Define degenerate orbitals.
(vii) Apply Hund's rule to explain why nitrogen has three unpaired electrons.
(viii) Write the behavior of protons and electrons in an electric field.

Q.3 Extensive Questions. **(2 × 4 = 8)**

(a) What are quantum numbers? Describe briefly principal and spin quantum numbers.
(b) Draw the shapes of s, p and d-orbitals. Justify these by keeping in view the azimuthal and magnetic quantum numbers.

Chapter 03 CHEMICAL BONDING

Student Learning Outcomes

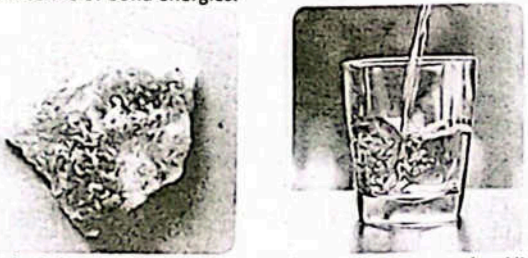
After studying this chapter, students will be able to:

- Analyze the formation of dative bond in CO, ozone and H_3O^+ ion (resonance structures are not required). **(Understanding)**
- Recognize that molecular ions/polyatomic ions can have expanded octets e.g., sulphate and nitrate. **(Understanding)**
- Use the differences in Pauling electronegativity values to predict the formation of ionic and covalent bonds. **(Application)**
- Use the concept of electronegativity to explain **bond polarity and dipole moments** of molecules. **(Understanding)**
- Explain the importance of **VSEPR theory** in the field of drug design by discussing how the shape and bond angles of the molecules help chemist predict their interactions in the body. **(Understanding)**
- Describe the shapes and bond angles in molecules using VSEPR theory (including describing sketching). **(Understanding)**
- Explain valence bond theory. **(Understanding)**
- Predict the shapes, and bond angles in molecules and ions. **(Understanding)**
- Describe covalent bonding in molecules using the concept of hybridization to describe sp, sp^2, and sp^3 orbitals. **(Understanding)**
- Explain hybridization and types of hybridization. **(Understanding)**
- Explain the salient features of molecular orbital theory (MOT). **(Understanding)**
- Explain the paramagnetic nature of oxygen molecule in the light of MOT. **(Understanding)**
- Calculate bond order of N_2, O_2, F_2, and He_2. **(Understanding)**
- Describe the types of van der Waals forces. **(Understanding)**
- Describe hydrogen bonding limited to molecules including ammonia and water. **(Understanding)**
- Use the concept of hydrogen bonding to explain the anomalous properties of water. **(Understanding)**
- Use bond energy values and the concept of bond length to compare the reactivity of covalent molecules. **(Application)**
- State that, in general, ionic, covalent, and metallic bonding are stronger than intermolecular forces. **(Understanding)**
- Define electronegativity as the power of an atom to attract electrons to itself. **(Knowledge)**
- Explain the factors influencing the electronegativities of elements in terms of nuclear charge, shielding by inner shells and subshells. **(Understanding)**
- Explain the trends in electronegativity across a period and down a group of the periodic table. **(Understanding)**

Chemical Bond

"A chemical bond is the force that holds together two or more atoms, molecules or ions"

- The properties of a substance depend on the type of the chemical bond between its atoms.
- The term chemical bond includes ionic, covalent, dative, metallic bonds, as well as intermolecular forces, i.e. van der Waals forces. However, being weak enough, van der Waals forces are usually not termed as pure chemical bonds.
- We shall discuss the types of bonds in the light of electronegativity and its effect on the nature of bonding, dipole moment, and polarity. Then, the modern bonding theories such as VSEPR, VBT, Hybridization, and MOT will be discussed in detail. The intermolecular forces, i.e. van der Waals forces will also be taken into account. Finally, a comparison of the chemical bonds and intermolecular forces will be presented in terms of bond energies.



NaCℓ has ionic bond and is solid, but water is a covalent compound and liquid

TYPES OF BONDING

Lewis concept of bonding gives a simple explanation of the formation of all types of bonds. According to this theory, atoms make bonds to complete their outermost shells to have noble gas-like configuration. This is mostly attained through the formation of an octet in the valence shell.

Ionic Bond

According to the Lewis theory, the ***ionic bond is formed by the complete transfer of electrons from one atom with low ionization energy to another atom with high electron affinity.***

- The Na atom ($_{11}Na = 2,8,1$) tends to lose the outermost electron to form $Na^+(2,8)$ ion, which has the electronic configuration of $_{10}Ne$, a noble gas nearest to it. Chlorine atom $C\ell(2,8,7)$ gains one electron to form the chloride ion, $C\ell^-(2,8,8)$, also gaining the next noble gas electron arrangement. The oppositely charged Na^+ and $C\ell^-$ ions are held together by strong ionic bond in the crystal of NaCℓ.
- A similar type of bond is expected between group 1and 2 metals and groups 16 and 17 elements.

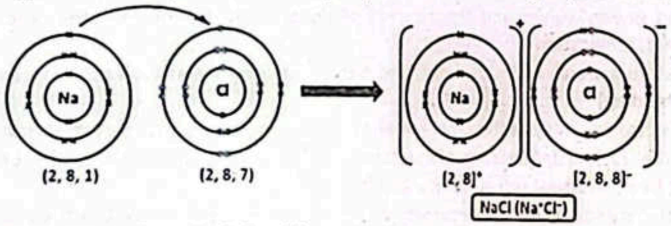


Figure: Ionic bond formation between Na and Cℓ

Covalent Bond (Electron Pair Bond)

- ***A covalent bond is formed by the mutual sharing of electrons between two atoms.***
- While sharing electrons, each atom completes its valence shell and attains the nearest noble gas configuration. The bond formation between two Cℓ atoms is shown below (Fig.).

- A covalent bond may be:
  (i) Non-polar in character **(ii) Polar in character.**
- The bond between two Cℓ atoms is purely covalent and non-polar. The electronegativity of the two atoms is exactly the same, due to which, the bonded atoms remain electrically neutral and there is no charge on either atom. The other such molecules are H_2, F_2, Br_2 and I_2.
- Examples of polar covalent bonds: $H-C\ell$, $H-Br$, H_2O, etc.

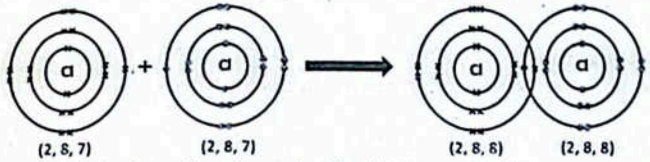


Figure: formation of a covalent bond between two Cℓ atoms

Rack Your Brain!

1. The bond which is formed by mutual sharing of electrons is called:
(A) Ionic bond
(B) Covalent bond
(C) Metallic bond
(D) Coordinate Covalent bond

Dative bond (Coordinate Covalent Bond)

Definition:

"A dative bond is formed between two atoms when the shared pair of electrons is donated by one of the bonding atoms".

Examples:

Rack Your Brain!

2. Justify that Covalent Bonds is directional in nature.

(a) Hydronium Ion

Let us consider the example of bond formation between H_2O and a proton (H^+).

- H_2O has two covalent bonds and there are two lone pairs of electrons on the oxygen atom.
- On the other hand, the proton is deficient in electrons. Therefore, the oxygen atom can donate its lone pair of electrons to the acceptor H^+, and this results in the formation of a dative bond as in the following diagram Figure (a).

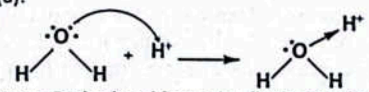
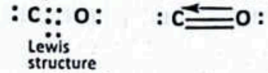


Figure : Dative bond formation (hydronium) ion,

(b) Carbon Monoxide

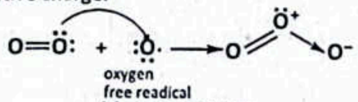
- Carbon monoxide also contains a dative bond between oxygen and carbon atoms.
- Oxygen shares its two valence shell electrons with the carbon atom to make normal double covalent bond. However, the valency of carbon is not satisfied with these bonds.
- It needs one more pair of electrons to complete its octet. Oxygen atom donates one of its lone pairs for the formation of a covalent bond, which is a dative bond as exhibited in Figure (b).



(b) Carbon monoxide

(c) Ozone Molecule

- The structure of ozone molecule is presented in Figure (c).
- It is formed by a reaction between the oxygen molecule with an oxygen atom (a free radical (O)).
- One of the oxygen atoms in the molecule donates a pair of electrons to make a coordinate covalent bond with this free radical.
- Therefore, the central atom has total three bonds including a double covalent bond on one side and a coordinate covalent bond on the other. It carries a positive charge, while the oxygen atom that accepts the lone pair carries a negative charge.



(c) ozone molecule

QUICK CHECK 3.1

a) Draw the Lewis structures of N_2 and CS_2 molecules?

Ans. N_2: :N≡N:

CS_2: :S̤: :C: :S̤:

b) How many electrons are there in the valence shell of B in BF_3? Does it have the ability to accept a lone pair of electrons?

Ans. In BF_3, the boron (B) atom has:

- 3 valence electrons (Group 13 element).
- Forms 3 bonds with fluorine (F), using all valence electrons (no lone pairs).

Ability to Accept Lone Pair:

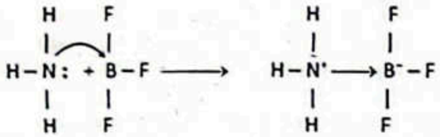
- Boron's valence shell has only 6 electrons (incomplete octet).
- Yes, it can act as a Lewis acid by accepting a lone pair (e.g., forming BF_4^- with F^-).

In short:

- Valence electrons in BF_3: 3 (all bonded).
- Electron-deficient, accepts lone pairs to complete octet.

c) Show the formation of a dative bond between NH_3 and BF_3.

Ans.

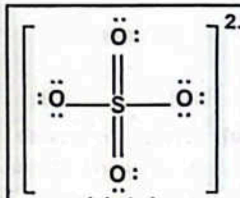


donor acceptor complex

Expanded Octet in Polyatomic Ions

Polyatomic ions are the ions composed of more than one type of atoms.

- There formal charge is the net charge on them which is calculated based on the number of electrons in their valence shells after the formation of bonds.
- With the exception of ammonium ion (NH_4^+), these ions mostly carry a negative charge, for example the carbonate (CO_3^{2-}), sulfate (SO_4^{2-}), and nitrate (NO_3^{1-}) ions.



sulphate ion

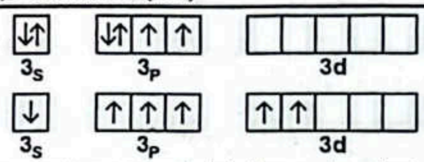
- In some polyatomic ions, the central atom violates the octet rule by expanding its electron density to the higher orbitals. These are said to have expanded octets.
- Examples: SO_4^{2-}, ClO_4^-, PO_4^{3-}.

> **Octet Rule:**
> The tendency of atoms to attain a maximum of eight electrons in the valence shell is known as the octet rule.

__Sulphate SO_4^{2-}:__

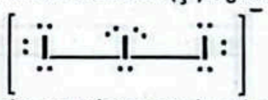
- From the Lewis structures of SO_4^{2-}, we can calculate the number of electrons around the central S atom.
- The number of electrons in the valence shell of S atom can be calculated as:
- No. of valence electrons= 2 × (double bond electrons) + 2 × (single bond electrons)

  = 2(4) + 2(2) = 12
- Thus, S has 12 electrons in its valence shell and it exceeds the octet by 4 electrons.
- The expansion of octet is caused by the involvement of the d orbital in bonding, which can accommodate the extra electrons. The following electronic configuration of native S(0) atom shows that it has two unpaired electrons in the p orbitals. The presence of d-orbital allows this configuration to extend to 4 unpaired electrons by the transfer of one electron from the 3 p pair. It explains not only the variable oxidation states of S, but also the possibility of accepting extra electrons in its d orbital.



> **Rack Your Brain!**
> 3. Octet rule is not followed in:
> (A) CH_4 (B) CF_4
> (C) CCl_4 (D) PCl_5

In the same way, we can calculate the number of valence electrons around the central iodine atom in the tri-iodide ion. The Lewis structure of the tri-iodide ion (I_3^{-1}) is given by:



The number of valence electrons of the central atom can be calculated as follows:

No. of valence electrons = 2 × (no. of single bond electrons) + 2 × (no. of lone pairs)

= 2(2) + 2(3)

= 10

The central iodine atom in tri-iodide ion (I_3^{-1}) has 10 electrons in the valence shell and the octet expands by two electrons.

QUICK CHECK 3.2

a) Can the elements of period 2 of the periodic table have expanded octet? Explain why or why not?

Ans. No, elements of Period 2 cannot have expanded octets because they lack the necessary orbitals to accommodate more than 8 electrons in their valence shell.

Detailed Explanation:

What is an "Expanded Octet"?

- An expanded octet refers to a situation where an atom has more than 8 electrons in its valence shell.
- This is possible only if the atom has access to empty d orbitals, which can be used to hold extra electrons beyond the typical s and p orbitals.

Electron Configuration of Period 2 Elements

Period 2 elements include:

Lithium (Li), Beryllium (Be), Boron (B), Carbon (C), Nitrogen (N), Oxygen (O), Fluorine (F), Neon (Ne)

- These elements have valence electrons in the second energy level (n = 2).
- The second energy level has the following orbitals:

  2s (1 orbital)

  2p (3 orbitals)
- Total: 4 orbitals → can hold a maximum of 8 electrons (4 × 2 electrons)

No d orbitals in Period 2

- d orbitals first appear in the 3rd period (n = 3).
- Since Period 2 elements don't have 3d orbitals, they are limited to the 2s and 2p orbitals only.
- Therefore, they cannot accommodate more than 8 electrons in their outer shell.

Examples:

Element	Normal Valency	Can It Expand Octet?	Why/Why Not?
Carbon (C)	4	No	$2s^2 2p^2$ → Max $8e^-$
Nitrogen (N)	3	No	$2s^2 2p^3$ → No d orbitals
Oxygen (O)	2	No	$2s^2 2p^4$ → Octet only
Fluorine (F)	1	No	$2s^2 2p^5$ → Can't exceed octet

Contrast with Period 3 and Beyond

- Starting from Period 3, elements like phosphorus (P), sulfur (S), chlorine (Cl) have access to 3d orbitals.
- This allows them to have expanded octets.