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International
AS & A Level

As notes

**M. SC
CHEMISTRY**

0300-4815012

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2 Atomic structure

This topic describes the type, number and distribution of the fundamental particles which make up an atom and the impact of this on some atomic properties.

Learning outcomes

Candidates should be able to:

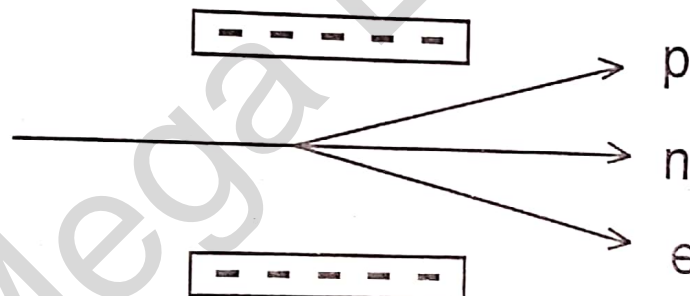
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- 2.1 Particles in the atom**
- a) identify and describe protons, neutrons and electrons in terms of their relative charges and relative masses
 - b) deduce the behaviour of beams of protons, neutrons and electrons in electric fields
 - c) describe the distribution of mass and charge within an atom
 - d) deduce the numbers of protons, neutrons and electrons present in both atoms and ions given proton and nucleon numbers (atomic and mass numbers) and charge
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- 2.2 The nucleus of the atom**
- a) describe the contribution of protons and neutrons to atomic nuclei in terms of proton (atomic) number and nucleon (mass) number
 - b) distinguish between isotopes on the basis of different numbers of neutrons present
 - c) recognise and use the symbolism ${}^A_Z\text{X}$ for isotopes, where A is the nucleon (mass) number and Z is the proton (atomic) number
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- 2.3 Electrons: energy levels, atomic orbitals, ionisation energy, electron affinity**
- a) describe the number and relative energies of the s, p and d orbitals for the principal quantum numbers 1, 2 and 3 and also the 4s and 4p orbitals
 - b) describe and sketch the shapes of s and p orbitals
 - c) state the electronic configuration of atoms and ions given the proton (atomic) number and charge, using the convention $1s^2 2s^2 2p^6$, etc.
 - d)
 - (i) explain and use the term *ionisation energy*
 - (ii) explain the factors influencing the ionisation energies of elements
 - (iii) explain the trends in ionisation energies across a period and down a group of the Periodic Table (see also Section 9.1)
 - e) deduce the electronic configurations of elements from successive ionisation energy data
 - f) interpret successive ionisation energy data of an element in terms of the position of that element within the Periodic Table
 - g) **explain and use the term *electron affinity***
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Atomic Structure

Sub atomic particles and their properties

Particles	Relative mass	Relative charge
Proton	1	+1
neutron	1	0
electron	$\frac{1}{1840}$	of the mass of proton -1

Behavior of proton electrons and neutrons in an electric field and a magnetic field



In an electric or magnetic field electrons are deflected towards the positive pole while protons are deflected towards the negative pole while neutrons do not deflect as they carry no charge.

Electronic configuration

- The arrangement of electrons in different shells and sub shells is called electronic configuration.
- Electrons are arranged in different shells and sub shells according to the increasing order of their energy.

Shell or orbit or energy level (n)

- ⇒ It is the path around the nucleus where electron revolves.
- ⇒ Orbits are represented by english alphabets K, L, M, N, O, P, Q, ...
- ⇒ The energy order of shells is $K < L < M < N < O < P < Q$

Principal quantum number

Each orbit is also represented by a number called principal quantum number e.g. Principal quantum number for K, L, M, N, O, P and Q is 1, 2, 3, 4, 5, 6 and 7 respectively

Sub shells: sub shells are the

sub division of shells.

- ⇒ There are four sub shells represented by s, p, d and f
- ⇒ Energy order of sub shells is $s < p < d < f$

orbitals: orbitals are the

sub-division of sub shells.

- ⇒ An orbital cannot accommodate more than 2 electrons

<u>sub shell</u>	<u>orbitals</u>
s	one (s)
p	three (p_x, p_y, p_z)
d	Five ($d_{xy}, d_{yz}, d_{zx}, d_{x^2-y^2}, d_{z^2}$)
f	seven

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<u>Shells</u>	<u>Sub shells</u>	<u>Number of electrons in each shell</u>
K	1s	2
L	2s 2p	8
M	3s 3p 3d	18
N	4s 4p 4d 4f	32
O	5s 5p 5d 5f	32
P	6s 6p 6d 6f	32
Q	7s 7p 7d 7f	32

<u>Sub shells</u>	<u>Electrons</u>
s	2
p	6
d	10
f	14

Rules for electronic configuration

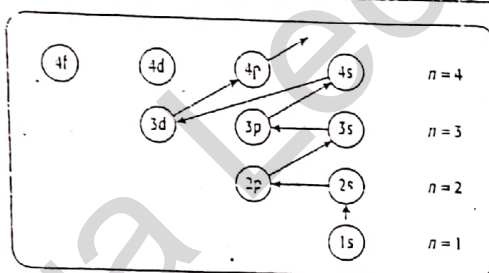
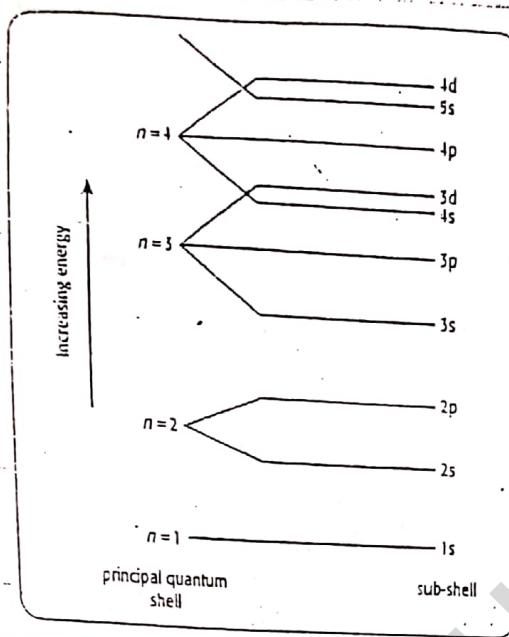
Auf Bau Principle :- According to this

principle, electrons are filled up in different shells and sub shells according to the increasing order of their energy.

e.g. 19K

$1s^2, 2s^2, 2p^6, 3s^2, 3p^6, 3d^2$ X Wrong
 $1s^2, 2s^2, 2p^6, 3s^2, 3p^6, 4s^2$ ✓ Correct

Energy of 4s is lower than 3d

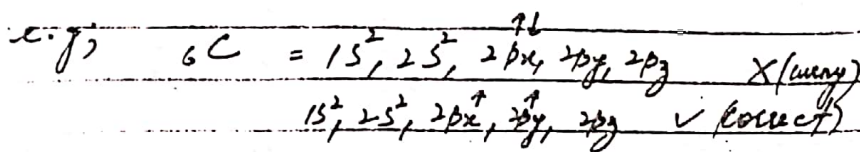


Pauli's exclusion principle: A orbital

cannot accommodate more than 2 electrons.

Hund's rule: If degenerate orbitals

(orbitals of same energy) are available then electrons would like to go in separate orbitals rather than in a same orbital.



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As the electrons are added they go into orbitals of increasing energy

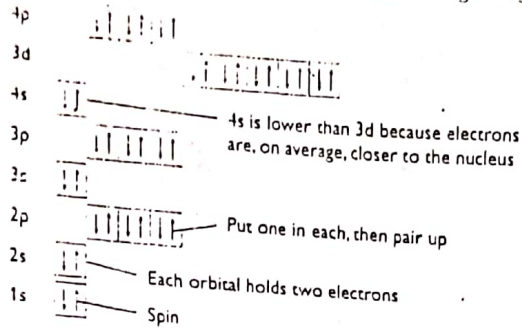
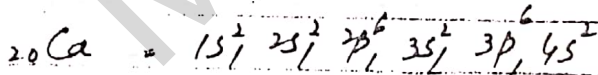
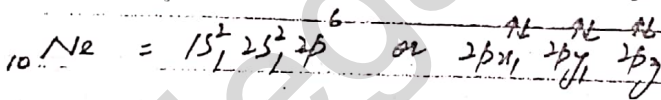
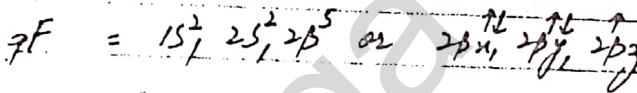
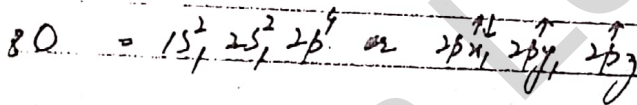
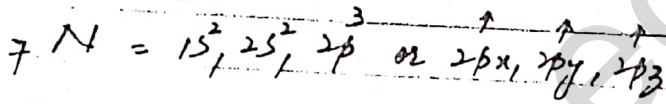
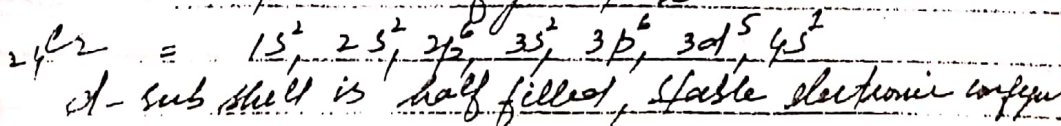
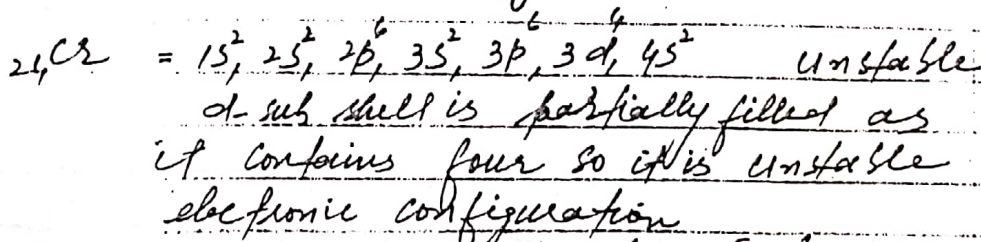


Figure 2.1 Sequence of filling orbitals with electrons

Examples of electronic configuration



Stable and unstable electronic configuration



Similarly $_{29}\text{Cu}$

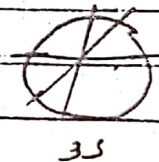
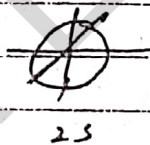
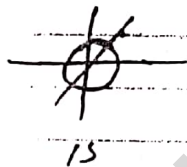
$1s^2, 2s^2, 2p^6, 3s^2, 3p^6, 3d^9, 4s^2$ Unstable

$1s^2, 2s^2, 2p^6, 3s^2, 3p^6, 3d^{10}, 4s^1$ Stable

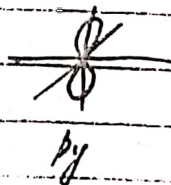
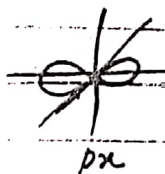
Shapes of orbital

s-orbitals :- s-orbitals are

spherical in shape and the size of sphere increases with the increase in shell number.



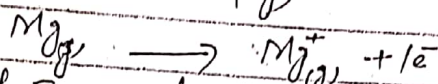
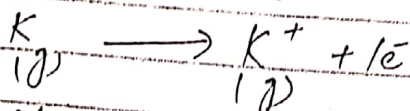
p-orbital :- p-orbitals are dumbbell or hourglass with two lobes.



Ionization energy

1st Ionization energy: Amount of energy

which is required to remove one mole of electrons from one mole of a gaseous atom to form ^{one mole of} monopositive gaseous ions e.g;



2nd Ionization energy: Amount of energy

which is required to remove one mole of electrons from one mole of monopositive gaseous ions to form one mole of dipositive gaseous ions, e.g;



Factors affecting ionization energy

(i) Shielding effect: Electrons present

between nucleus and valence shell protect valence electrons from nuclear attraction, this is called shielding effect.

⇒ Increase in shielding effect decreases the ionization energy by decreasing the effective nuclear charge and by

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decreasing - the attraction between nucleus and valence electrons

(2) Nuclear charge and effective nuclear charge

Nuclear charge :- Total number of

protons present in the nucleus of an atom is called nuclear charge.

Effective nuclear charge: Total

number of protons minus number of inner shell electrons is called effective nuclear charge

^{11}Na

$$11p - 10e = +1 \text{ (effective nuclear charge)}$$

^{12}Mg

$$12 - 10 = +2 \text{ effective nuclear charge}$$

^{13}Al

$$13 - 10 = +3 \text{ effective nuclear charge}$$

⇒ presence of inner shell electrons cancels the nuclear attraction for valence electrons but not completely.

⇒ Increase in nuclear charge or effective nuclear charge both increase the ionization energy by increasing attraction between nucleus and valence and by pulling valence shell

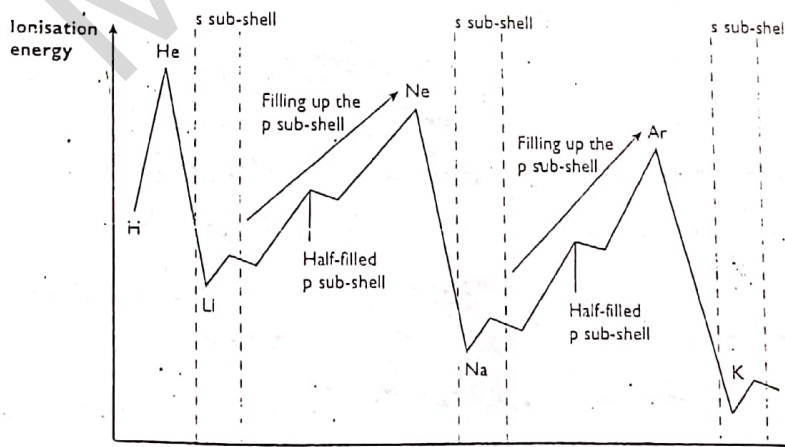
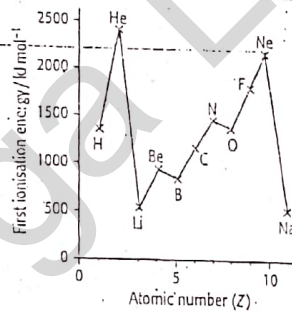
more towards the nucleus.

Trends in Ionization energy

Across the period: 1st ionization

energy increases from left to right across the period due to the following reasons.

- ⇒ Effective nuclear charge increases from left to right across the period
- ⇒ Shielding effect remains constant
- ⇒ atomic size decreases
- ⇒ due to this valence electron(s) get closer to the nucleus, hence more energy will be required to remove electrons.



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Along the group

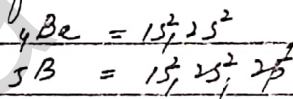
Unusual trends in ionization energy across the period

i) From group II to III :- 1st Ionization energy

decreases from group II to group III due to the difference in valence sub shell
 ⇒ group III elements have their valence electrons in p-sub shell while group II elements have valence electrons in s-sub shell

⇒ p-sub shell is at higher energy or electrons in p-sub shell are at higher energy

⇒ group II elements have completely filled s-sub shell, so more difficult to remove electron from s-sub shell of group II e.g.;

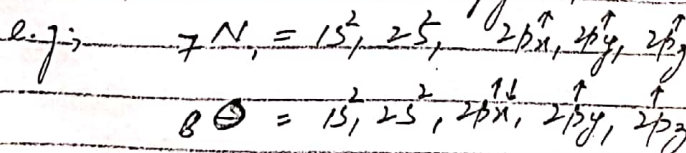


ii) From group V to VI :- 1st ionization

energy of group V elements is greater than that of group VI due to the following reasons

i) Group V elements have half filled p-sub shell which is more stable than partially filled p-sub shell of group VI

ii) pair of electrons in p-sub shell of group VI repel each other and need lesser energy to remove



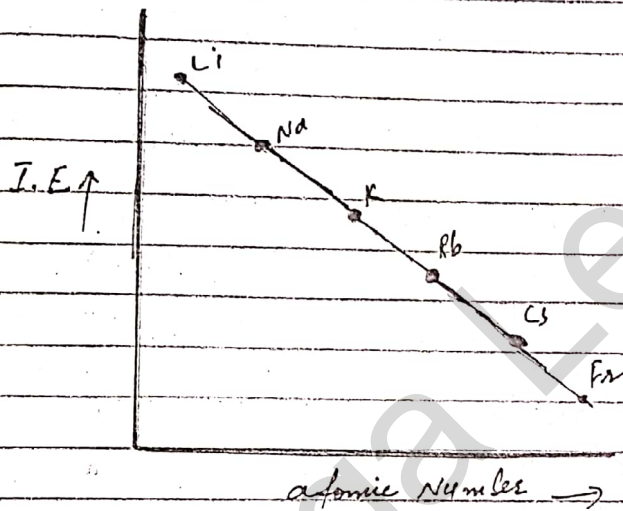
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(2) Along the group

Ionization energy decreases down the group due to following reasons

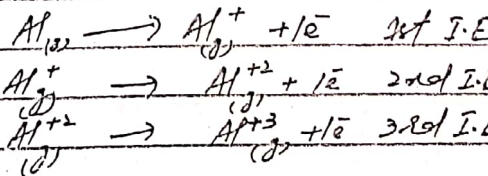
⇒ Increase in atomic size due to the increase in number of shells decreases the electrostatic attraction between nucleus and valence electrons.

⇒ Increase in shielding effect



Successive Ionization energy

Successive ionization energy refers to the removal of 2nd and subsequent electrons e.g;



Prediction of group number

Successive ionization energies of an unknown element can help predict

the group number of that element.
Successive ionization energies increase as the outer electrons are removed and biggest jump occurs when an electron is removed from a new inner orbital closer to the nucleus.

For example, the five successive ionization energies of an unknown element are given, predict the group number of that element

1st I.E	2nd I.E	3rd I.E	4th I.E	5th I.E
578	1817	2744	11577	14822

Biggest Increase

Biggest increase from 3rd to 4th I.E indicates the change in orbitals, so element is present in group III and have three valence electrons.

Similarly

1st I.E	2nd I.E	3rd I.E	4th I.E	5th I.E
598	1145	4912	6491	8153

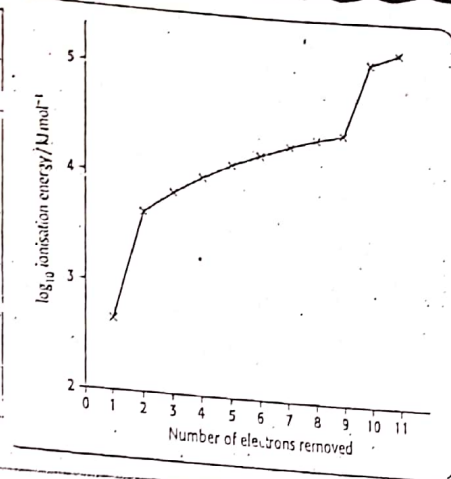
Biggest increase

Biggest increase from 2nd to 3rd I.E indicates the presence of element in group II.

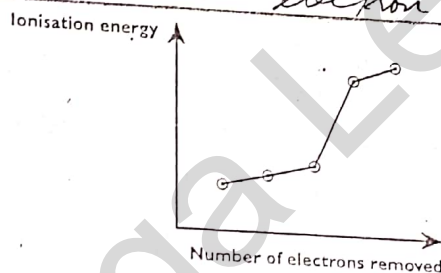
1st I.E	2nd I.E	3rd I.E	4th I.E	5th I.E
496	4562	6910	9543	13354

Biggest increase (group I)

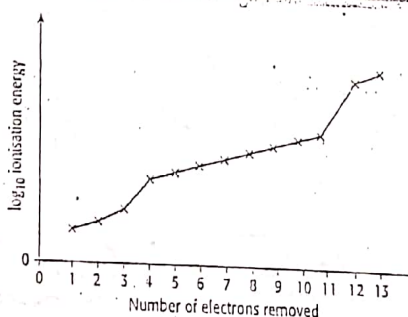
A graphical representation of successive ionization energies and prediction of group number



Biggest difference between 1st and 2nd ionisation energy indicates the change in shell, so group I, one valence electron



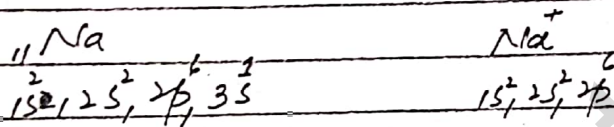
Biggest difference between 3rd and 4th, so third group



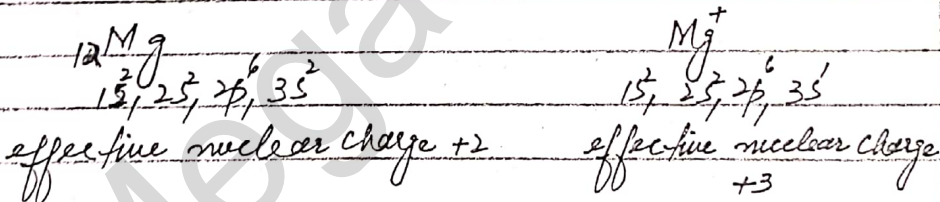
Biggest difference between 3rd and 4th so 3rd group.

Why 2nd ionization energy is greater than 1st?

For group I elements, 2nd electron is removed from the inner shell i.e; 2nd shell which is closer to the nucleus. Secondly after the removal of one electron effective nuclear charge increases which increases the electrostatic attraction between nucleus and valence electron.



⇒ For other elements removal of one electron increases effective nuclear charge, as a result nucleus have stronger hold over remaining electrons.



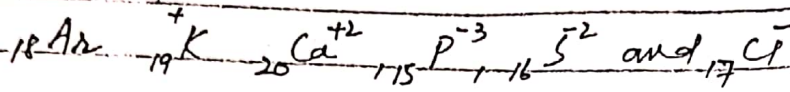
Important Note:

Increase in protons in the nucleus or removal of electron from the shell, both increase effective nuclear charge

Radii of isoelectronic substances

Isoelectronic: substances with same number of electrons are called isoelectronic.

For example



- ⇒ All have same number of electrons and are isoelectronic
- ⇒ Ca^{+2} has greatest effective nuclear charge and smaller radii
- ⇒ P^{-3} has lowest effective nuclear charge and has largest radii
- ⇒ So Ca^{+2} will have highest 1st I.E.

Another example

	$_{10}\text{Ne}$	$_{8}\text{O}^{-2}$	$_{9}\text{F}^{-1}$	$_{11}\text{Na}^+$	$_{12}\text{Mg}^{+2}$	$_{13}\text{Al}^{+3}$
Radii		0.14	0.133	0.102	0.072	0.053

- ⇒ Al^{+3} has greatest effective nuclear charge and smallest radii, so highest 1st I.E.
- ⇒ O^{-2} has lowest effective nuclear charge and greatest radii, so have lowest 1st ionization energy.