CHAPTER 1
Atomic Structure

Learning Outcomes

Candidates should be able to:

(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 an electric field

(c) describe the distribution of mass and charges within an atom

(d) deduce the numbers of protons, neutrons and electrons present in both atoms and ions given proton and nucleon numbers (and charge)

(e) (i) describe the contribution of protons and neutrons to atomic nuclei in terms of proton number and nucleon number

(ii) distinguish between isotopes on the basis of different numbers of neutrons present

(f) 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

(g) describe the shapes of s, p and d orbitals

[knowledge of wave functions is **not** required]

(h) state the electronic configuration of atoms and ions given the proton number (and charge)

(i) explain the factors influencing the ionisation energies of elements (see the Data Booklet)

(j) deduce the electronic configurations of elements from successive ionisation energy data

(k) interpret successive ionisation energy data of an element in terms of the position of that element within the Periodic Table

<u>Trends and variations in atomic and physical properties</u>

For elements in the third period (sodium to chlorine), and in Group 2 (magnesium to barium) and Group 17 (chlorine to iodine) candidates should be able to:

(l) recognise variation in the electronic configurations across a Period and down a Group

(m) describe and explain qualitatively the trends and variations in atomic radius, ionic radius, first ionisation energy and electronegativity:

(i) across a Period in terms of shielding and nuclear charge

(ii) down a Group in terms of increasing number of electronic shells and nuclear charge

(n) define the terms *relative atomic*, *isotopic*, *molecular* and *formula mass*, based on the ^{12}C scale

(o) calculate the relative atomic mass of an element given the relative abundances of its isotopes

(p) explain what is meant by a transition element, in terms of d block elements forming one or more stable ions with partially filled d subshells

(q) state the electronic configuration of a first row transition element and its ions

(r) explain why atomic radii and first ionisation energies of the transition elements are relatively invariant

PROPERTIES OF THE 3 SUBATOMIC PARTICLES

Property	Proton	Electron	Neutron
Relative charge	+1	–1	0
Relative mass	1	$\frac{1}{1836}$	1

Atom: The smallest component of an element having the chemical properties of the element

Isotopes: Atoms of an element that have the same proton number but different nucleon numbers

Proton number: The number of protons in the nucleus of each atom of an element

Nucleon number: The total number of neutrons and protons in the nucleus of an atom of an element

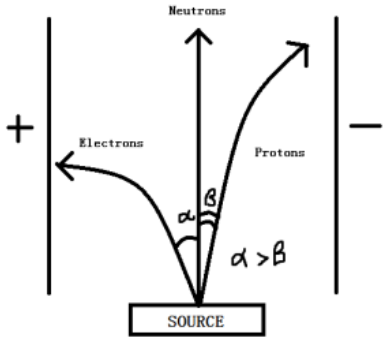
Deflection of charged particles

$\theta \propto \frac{q}{m}$

Isotopic → Same number of protons

Isotonic → Same number of neutrons

Isoelectronic → Same number of electrons



Relative atomic mass, A_r: Average mass of 1 atom of an element compared with $\frac{1}{12}$ the mass of 1 atom of ^{12}C

Relative isotopic mass: Average mass of 1 atom of an isotope of an element compared with $\frac{1}{12}$ the mass of 1 atom of ^{12}C

Atomic orbital: Region of space with a 90% probability of finding an electron

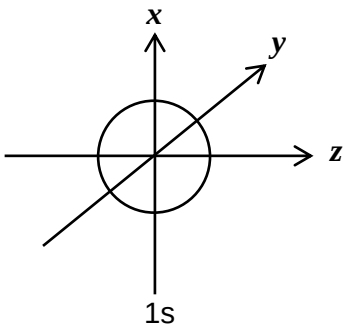
RELATIVE ABUNDANCE OF ISOTOPES

The A_r of Boron, which consists of the isotopes ^{10}B and ^{11}B is 10.8. What is the percentage of ^{11}B atoms in the isotopic mixture?
Let a be the relative abundance of ^{11}B atoms. Relative abundance of ^{10}B atoms is (1 – a). a(11) + (1 – a)(10) = 10.8 a = 0.8 so % of ^{11}B atoms in the mixture = 80.0%

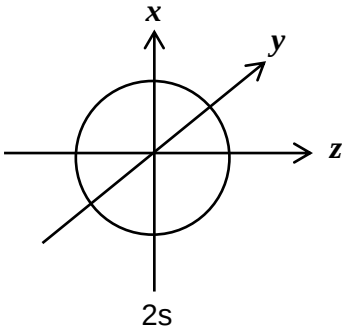
Summary of the relationship between principal quantum shells, subshells and orbitals

Principal quantum no.	Subshell	No. of orbitals	Max no. of e^- in each principal quantum shell
1	1s	1	2
2	2s 2p	1 3	8
3	3s 3p 3d	1 3 5	18
4	4s 4p 4d 4f	1 3 5 7	32

s Orbitals

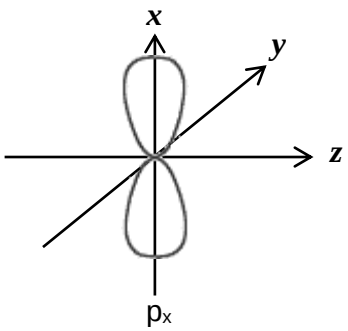


1s

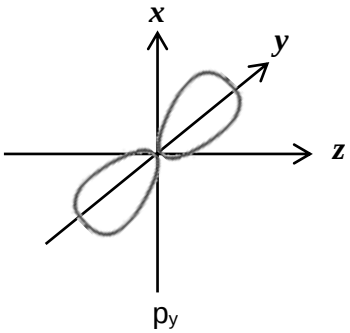


2s

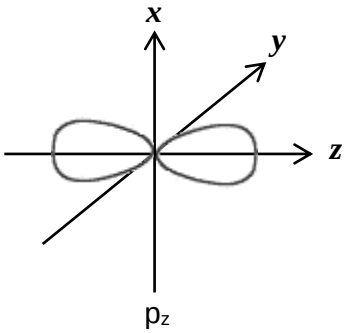
p Orbitals



p_x

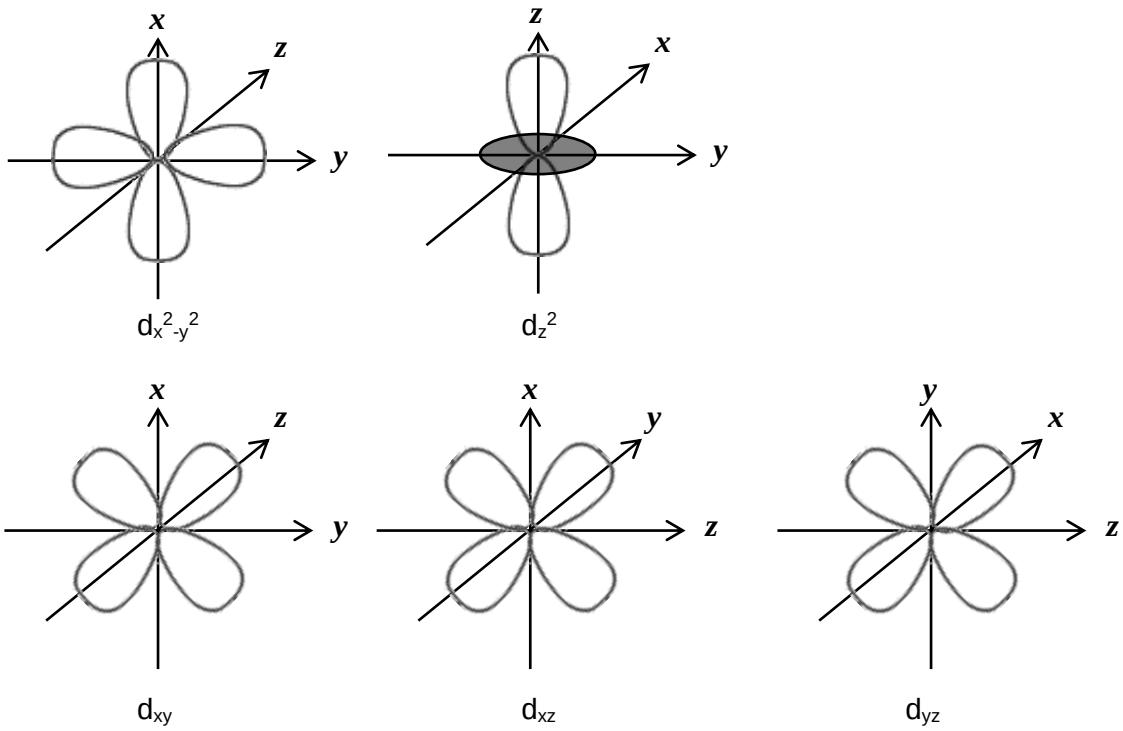


p_y



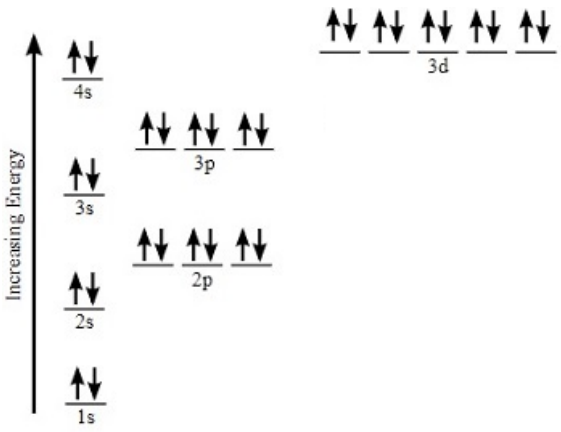
p_z

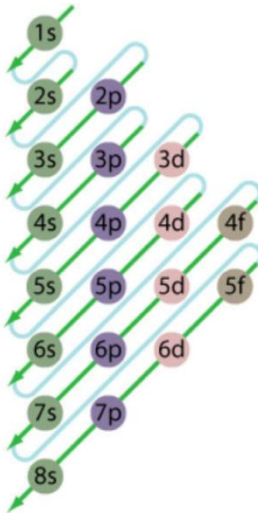
d Orbitals



1. Aufbau Principle

Electrons in their ground states occupy orbitals in order of energy levels





2. Hund's Rule of Multiplicity

When filling subshells that contain >1 orbital with the same energy, each orbital must be singly occupied before electrons are paired.

3. Pauli Exclusion Principle

An orbital can't hold >2 electrons and the 2 electrons sharing the same orbital must have opposite spins

Exceptions

Chromium: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^5\ 4s^1$

Copper: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^{10}\ 4s^1$

Cations: Remove electrons from the outermost subshell

Anions: Add electrons to the lowest energy orbital

Exceptions

Scandium forms Sc^{3+} which has the $3d^0$ configuration

Zinc forms Zn^{2+} which has the $3d^{10}$ configuration

TRENDS IN ATOMIC RADIUS

Increases down the group

- Number of quantum shells increases as more electrons are added to a new principal quantum shell
- Outermost electrons are further away from nucleus
- Although nuclear charge increases due to the increase in number of protons, the number of quantum shells is the more important factor

Decreases across the period

- Nuclear charge increases due to increasing number of protons
- Shielding effect remains relatively constant as electrons are added to the same outermost shell
- Effective nuclear charge increases, resulting in stronger electrostatic forces of attraction between nucleus and outermost electron so it is pulled closer to the nucleus

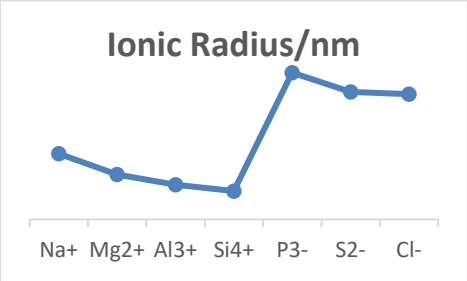
Relatively invariant across transition elements

- Nuclear charge increases due to increasing number of protons
- Shielding effect increases as electrons are added to the inner 3d subshell
- Shielding effect nullifies, to a considerable extent, the influence of each additional proton in the nucleus
- Effective nuclear charge remains almost constant

TRENDS IN IONIC RADIUS

Decrease in ionic radius across the cations and anions

- Na^+, Mg^{2+} and Al^{3+} are isoelectronic as they have the same number of electrons (10)
- P^{3-}, S^{2-} and Cl^- are isoelectronic as they have the same number of electrons (18)
- Across the 2 isoelectronic series, nuclear charge increases due to increasing number of protons
- Shielding effect remains the same due to the same number of electrons
- Increase in effective nuclear charge and stronger attraction between outermost electron and nucleus
- Sharp increase in ionic radius from cationic to anionic series is due to the anions having 1 more quantum shell than cations despite their higher nuclear charge



1st ionisation energy: Energy needed to remove 1 mole of electrons from 1 mole of gaseous atoms to form 1 mole of unipositively charged gaseous ions

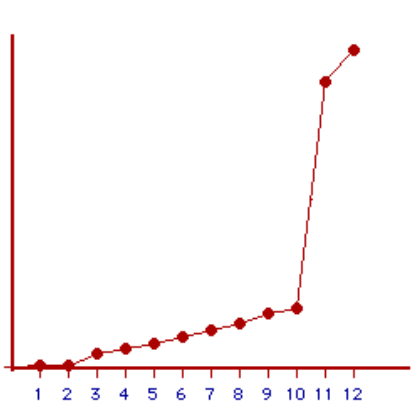
$$\mathbf{X\ (g) \rightarrow X^+\ (g) + e^-}$$

Ideal gas has negligible IMF so no extra energy is needed to overcome IMF, only for 1st I.E.

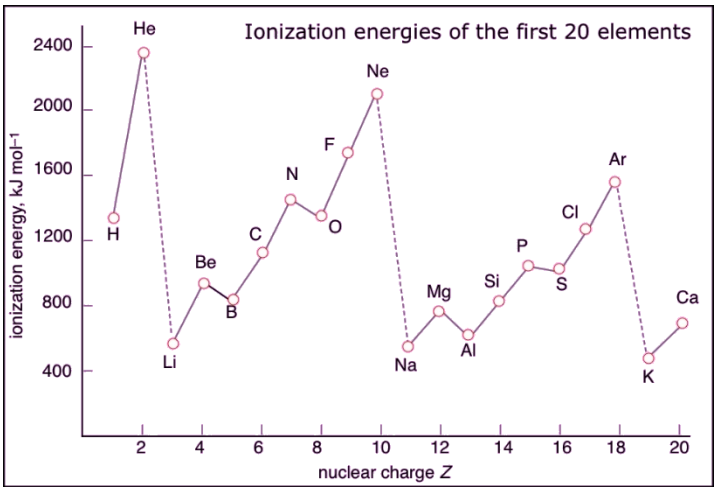
2nd ionisation energy: Energy needed to remove 1 mole of electrons from 1 mole of unipositively charged gaseous ions to form 1 mole of gaseous ions with double positive charge

$$\mathbf{X^+\ (g) \rightarrow X^{2+}\ (g) + e^-}$$

Successive Ionisation Energies of Mg



1st	737.7
2nd	1450.7
3rd	7732.7
4th	10542.5
5th	13630
6th	18020
7th	21711
8th	25661
9th	31653
10th	35458
11th	169988
12th	189367.7



- 1st big increase from 2nd to 3rd ionisation energies implies that the 3rd electron is in an inner quantum shell so there are 2 electrons in the valence 3s subshell → Mg is a Group 2 element
- Gradual increase from 3rd to 10th ionisation energies implies that the next 8 electrons are removed from the 2nd quantum shell
- Slightly greater increase from 8th to 9th ionisation energies as more energy is needed to remove the 2s electrons which are closer to the nucleus than the 2p electrons
- 2nd big increase from 10th to 11th ionisation energies implies that the last 2 electrons are in the 1st quantum shell

TRENDS IN IONISATION ENERGY

Decreases down the group

- Despite the increase in nuclear charge due to more protons, increase in number of quantum shells of electrons means that the outermost electrons are further from the nucleus
- Electrostatic forces of attraction between the nucleus and the outermost electron are weaker so less energy is needed to remove an electron

Increases across the period

- Nuclear charge increases due to increasing number of protons
- Shielding effect remains relatively the same as electrons are added to the same principal quantum shell
- Effective nuclear charge increases and electrostatic forces of attraction between outermost electrons and nucleus become stronger so more energy is needed to remove an electron

EXCEPTIONS

Small dip between Group 2 and 13 elements

- 3p subshell of A*l* is further away from the nucleus than the 3s subshell of Mg
- Weaker attraction between outermost electrons and nucleus so lesser energy needed to remove the 3p electron from A*l*

Small dip between Group 15 and 16 elements

- P: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^3$
- S: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^4$
- All the 3p electrons in P are unpaired but in S, 2 of the 3p electrons are paired
- There is some inter-electronic repulsion between the paired electrons in the 3p subshell in S so lesser energy is need to remove 1 of these paired electrons from S

Relatively invariant across transition elements

- Nuclear charge increases due to increasing number of protons
- Shielding effect increases as electrons are added to the inner 3d subshell
- Shielding effect nullifies, to a considerable extent, the influence of each additional proton in the nucleus
- Effective nuclear charge remains almost constant

END