Notes on AS Chemistry 9701

Atomic Structure and Ionization Energies

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Atomic Structure

p	+1	1
n	0	1
e	−1	1/1836
	relative charge	relative mass

1 } $\rightarrow$ 1.67×10^{-27} Kg

} rounded value, not exactly 1

↳ relative to $\frac{1}{12}$ th the mass of ^{12}C

actual charge
1.6×10^{-19} Coulombs
(rounded value)

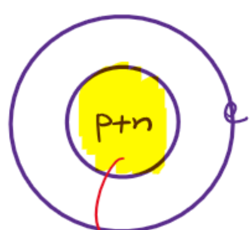
* mass is always in decimals, depends on accuracy.

measurable quantities → possible infinite significant figures.

basic model of an atom

Hydrogen

smallest atom
very stable
92% of the universe



electrons are in shells.

+ve nucleus
(nucleus attracts e−).

$2n^2$ → Total no. of e− in a shell

shell 1	(K)	2e max
shell 2	(L)	8e max
shell 3	(M)	18e max
shell 4	(N)	32e max
shell 5	(O)	50e max

nucleon no vs relative atomic mass

total no of (p+n)
* always a whole number
* never write in decimals.

average mass of an atom (including isotopes) of an element compared to ^{12}C

11p, 11e, 12n → 23.03

11×0.9986 — 10.98

0.0005439×11

12×1 — 12

$^{23}_{11}Na$

atomic no / proton no.
(for neutral atom equal to electron no.)

proton no defines element and its properties

Isotopes.

Atoms of same element having same proton no. (or atomic no.) but different no of neutrons (nucleon no.)

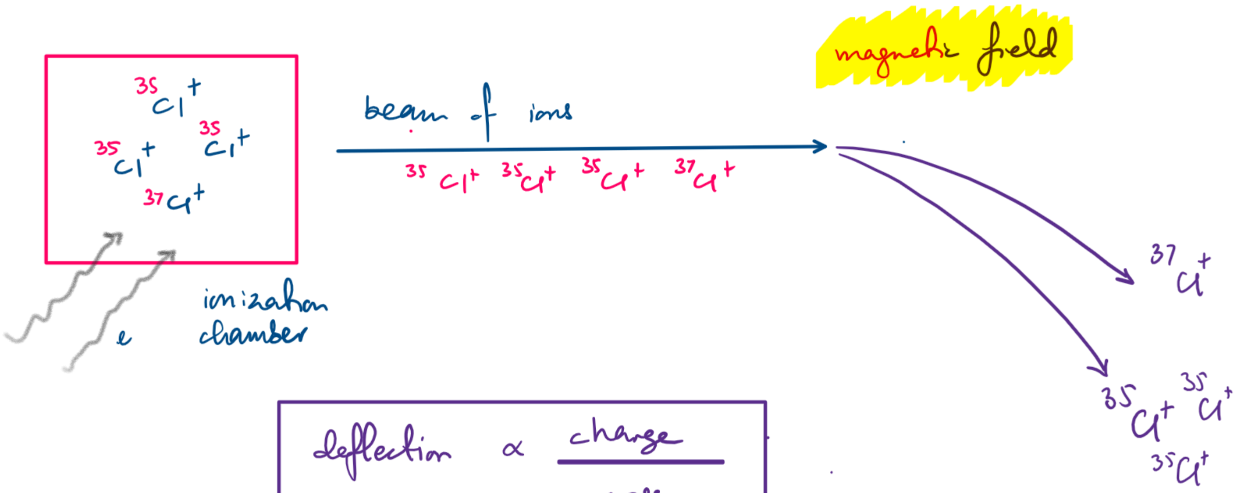
* don't use the word atomic mass

Relative Isotopic mass.

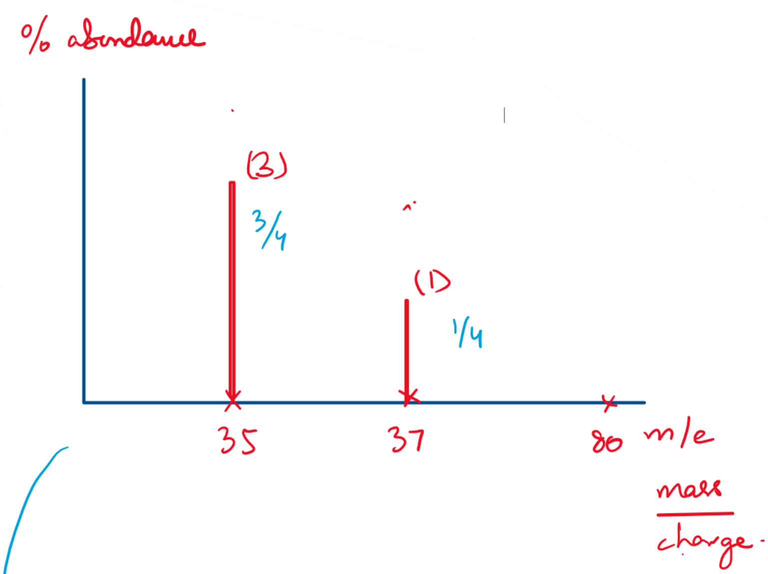
mass of an isotope of an atom compared to 1/12th the mass of ^{12}C

Calculate Relative Atomic mass .

mass spectroscope .



$$\boxed{\text{deflection} \propto \frac{\text{charge}}{\text{mass}}}$$

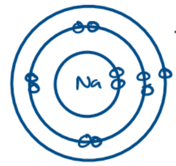


(not nucleon no)

$$A_r = \sum_{\text{Sum}} \frac{\% \times \text{isotopic mass}}{100} \;. \quad = \sum \text{fractional \%} \times \text{isotopic mass.}$$

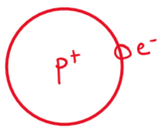
Electronic Configurations

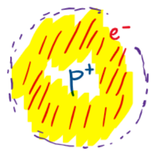
$^{23}_{11}Na$ 11p, 11e, 12n → 2, 8, 1



Orbitals

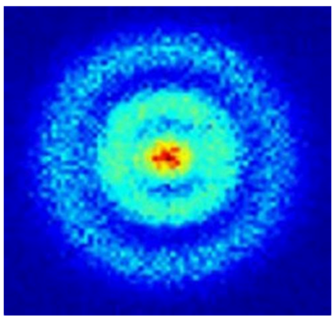
region in space where there is a high probability of finding an electron



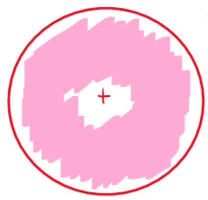


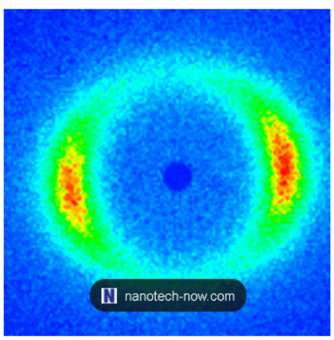
particle
exact mass, exact charge

wave
not well defined location

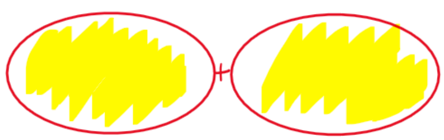


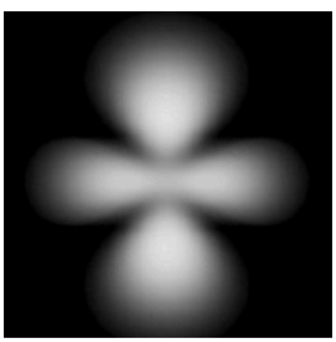
s-orbital · spherical region around the nucleus



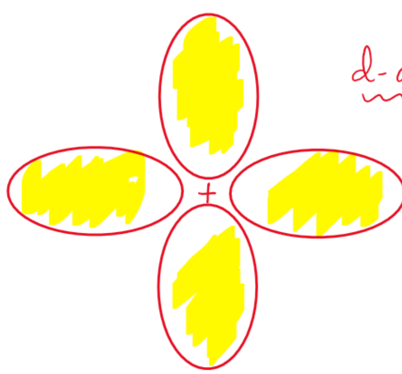


p-orbital - dumbell shaped



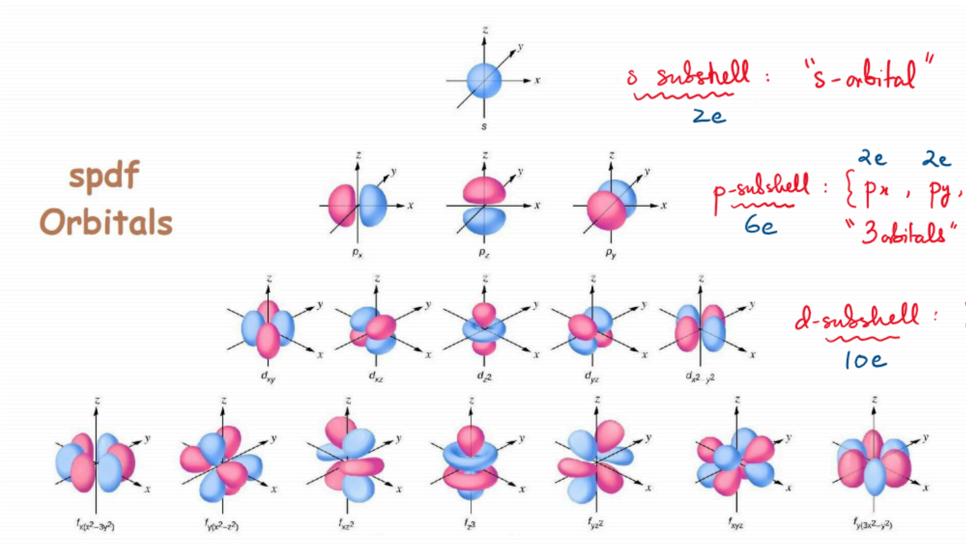


d-orbital



subshells .

group of degenerate orbitals
- same type
- same energy level



s subshell : "s-orbital"
2e

p-subshell : { p_x , p_y , p_z } (2e, 2e, 2e)
6e
"3 orbitals"

d-subshell : { d_{xy} d_{xz} d_{yz} $d_{x^2y^2}$ d_{z^2} }
10e
"5 × orbitals"

f-subshell : "7 × f orbitals"
14e

Orbital : maximum 2e .

both e⁻ have opposite spin

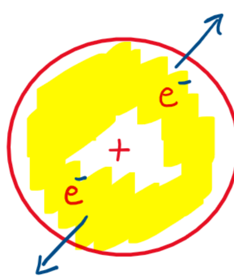
magnetic dipole / spin.

electron

S^2

$\boxed{\uparrow\downarrow}$.

arrows represent electrons , opposite spin



electrostatic repulsion

opp. magnetic spin attracts.

× hence force of repulsion cancels out.

Shells — Principal Quantum No

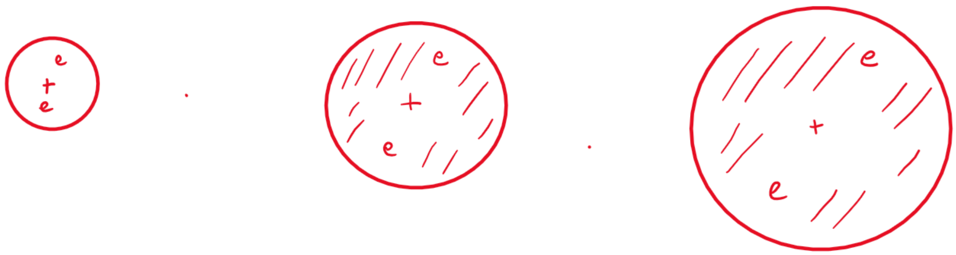
Energy level.

shell 1 — lowest energy level
shell 2 — (increase)
shell 3
⋮

$1s^2$ — no. of e^- — shell no. 1

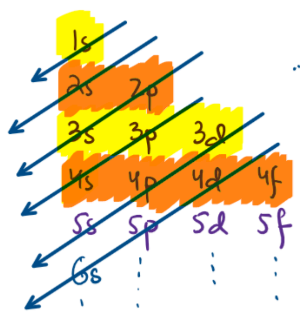
$2s^2$ — shell 2

$3s^2$ — shell 3. — subshell



"$2n^2$"
2e
8e
18e
32e
⋮

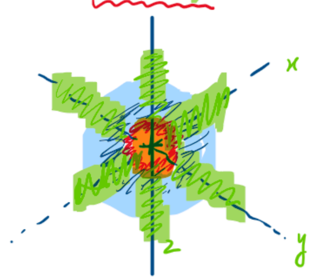
Aufbau Principal.

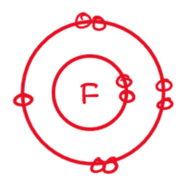


order of subshells

1s 2s 2p 3s 3p 4s ✓ 3d ✓ 4p 5s 4d 5p 6s

$_9F$ $1s^2$, $2s^2$, $2p^5$ → $2p_x^2$ $2p_y^2$ $2p_z^1$





* within a shell

s < p < d < f

e.g 3s < 3p < 3d

$_{26}Fe$ $\underbrace{1s^2}_{2e}$, $\underbrace{2s^2, 2p^6}_{8e}$, $\underbrace{3s^2, 3p^6, 3d^6}_{14e}$, $\underbrace{4s^2}_{2e}$

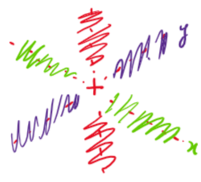
$_{19}K$ $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^1$

$_{8}O$ $1s^2\ 2s^2\ 2p^4 \rightarrow 2p_x^2\ 2p_y^1\ 2p_z^1$

$_{14}Si$ $1s^2,\ 2s^2\ 2p^6\ 3s^2\ 3p^2$

$3p_x^1\ 3p_y^1\ 3p_z^1$

e⁻ in a subshell always fill in a single manner



$3d^6 \{ 3d_{xy}^2\ 3d_{xz}^1\ 3d_{yz}^1\ 3d_{x^2-y^2}^1\ 3d_{z^2}^1 \}$

$_{19}K$ $1s^2,\ 2s^2,\ 2p^6,\ 3s^2,\ 3p^6,\ 4s^1$

$_{13}Al$ $1s^2,\ 2s^2,\ 2p^6,\ 3s^2,\ 3p^1$

$_{6}C$ $1s^2,\ 2s^2,\ 2p^2$

$\rightarrow 2p_x^1,\ 2p_y^1,\ 2p_z^0$

Two Special Cases.

$_{29}Cu$ $1s^2,\ 2s^2,\ 2p^6,\ 3s^2,\ 3p^6,\ \cancel{3d^9},\ \cancel{4s^2}$

$3d^{10},\ 4s^1$

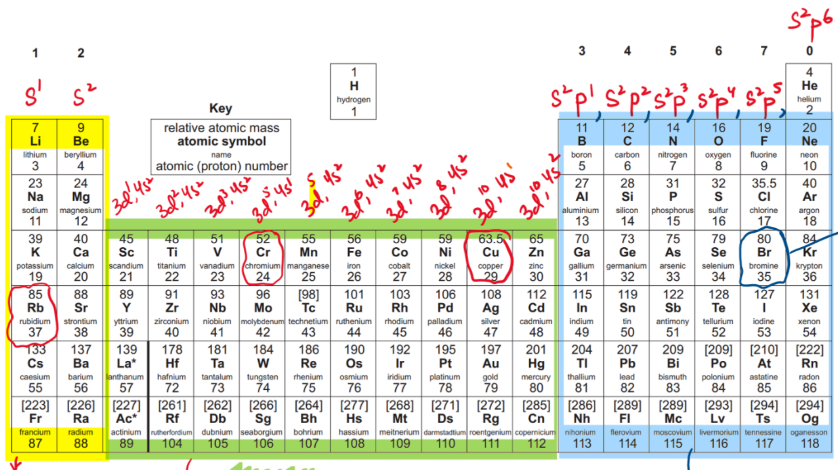
$_{24}Cr$ $1s^2,\ 2s^2,\ 2p^6,\ 3s^2,\ 3p^6,\ \cancel{3d^4},\ \cancel{4s^2}$

$3d^5,\ 4s^1$

Period Number tells you the total number of Shells while the Group Number tells you the Outer shell E-configuration.

Period No = Shell No.

$p_x^2\ p_y^1\ p_z^1$



$4s^2, 4p^5$

$1s^2, 2s^2, 2p^6, 3s^2, 3p^6, 3d^{10}, 4s^2, 4p^5$

s-block

d-block

P-block
last e⁻ goes into p.

Group No. = No. of Valence e⁻
Outershell e⁻ configuration

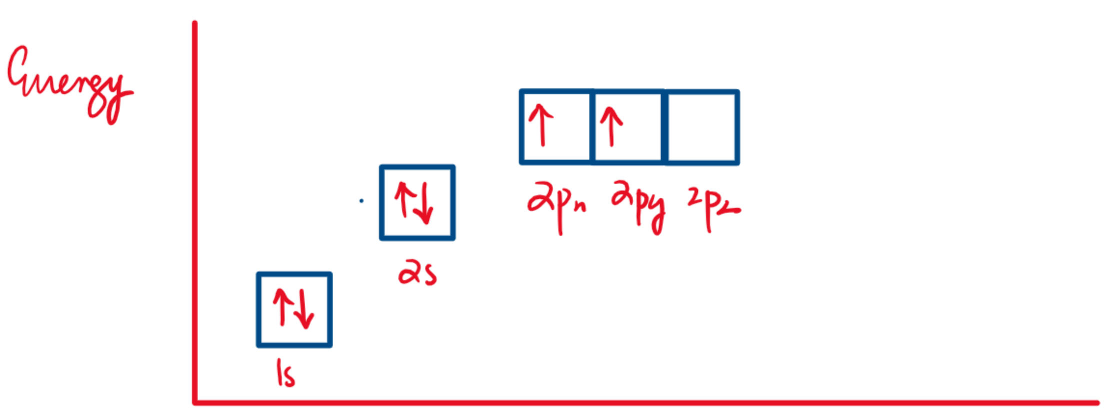
$_{37}Rb$ $1s^2, 2s^2, 2p^6, 3s^2, 3p^6, 3d^{10}, 4s^2, 4p^6, 5s^1$

$_{25}Mn$ $1s^2, 2s^2, 2p^6, 3s^2, 3p^6, 3d^5, 4s^2$

ions : e⁻ are removed from outer most shell

Block represenation for writing E-configuration

$_6C$ $1s^2, 2s^2, 2p^2$



Size of atoms / ions

Isoelectronic atoms

→ same no. of electrons

$_{11}Na^{+1}$ $\quad$ $_{10}Ne$ $\quad$ $_{8}O^{2-}$

$_{11}Na^{+1}$	$_{10}Ne$	$_{8}O^{2-}$
10e	10e	10e
11p	10p	8p.

nucleus has more protons
more attraction for e⁻
hence smaller

size of atoms down the group

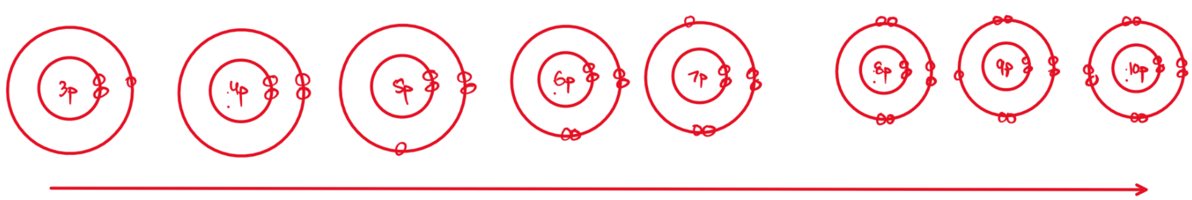
size increases
more shells

Li 2,1

Na 2,8,1

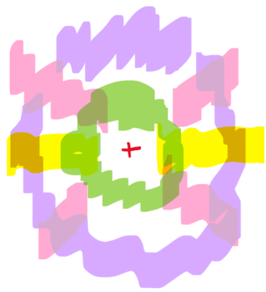
K 2,8,8,1

Across the period.



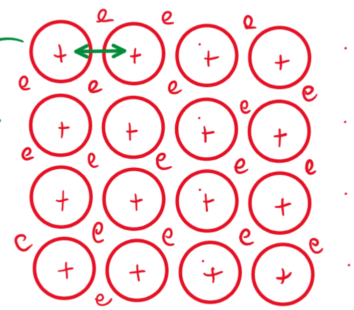
same shielding
increasing nuclear charge
more attraction for valence e⁻
smaller atomic radii

How are atomic radii measured.



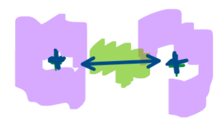
atom size is not well defined.

atomic radii = $\frac{\text{distance b/w nuclei}}{2}$



metal.

Cl$_2$ molecule

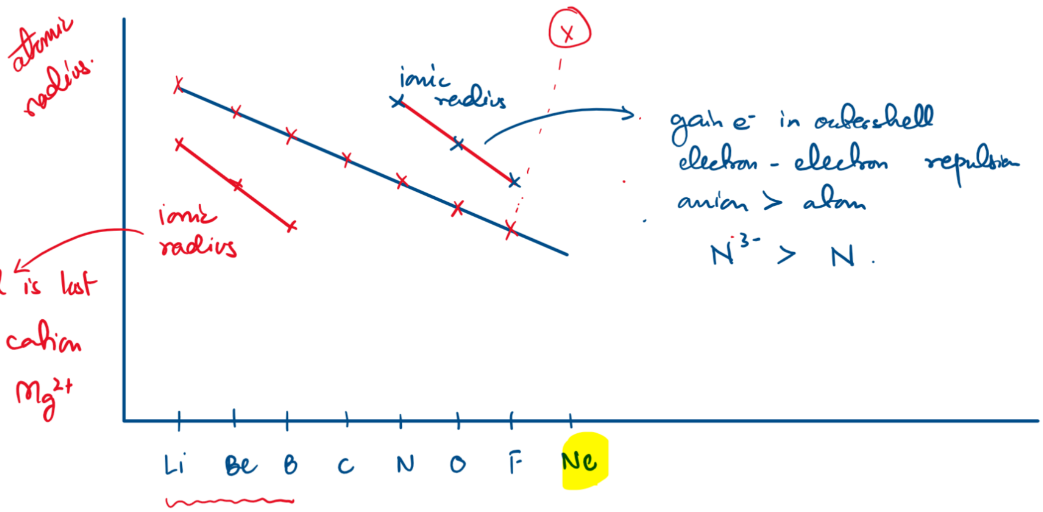


covalent molecules

Atomic radius is measured using distance between nuclei and dividing it by two since the atom's outer boundary is not well defined. For metals a metallic lattice is used and for nonmetals covalent molecules are used. Since noble gases don't bond, hence their atomic radii are incorrectly measured.

Noble gases / Ar or Ne
don't form bonds

atomic
radii incorrectly
measured.



gain e⁻ in outershell
electron - electron repulsion
anion > atom
$N^{3-} > N$.

outershell is lost
atom > cation
$Mg > Mg^{2+}$

Ionization Energy

$Na_{(g)} \longrightarrow Na^{+}_{(g)} + 1e$ 1st Ionization Energy

$Na^{+1}_{(g)} \longrightarrow Na^{+2}_{(g)} + 1e$ 2nd Ionization Energy.

$Na^{+7}_{(g)} \longrightarrow Na^{+8}_{(g)} + 1e$ 8th Ionization Energy

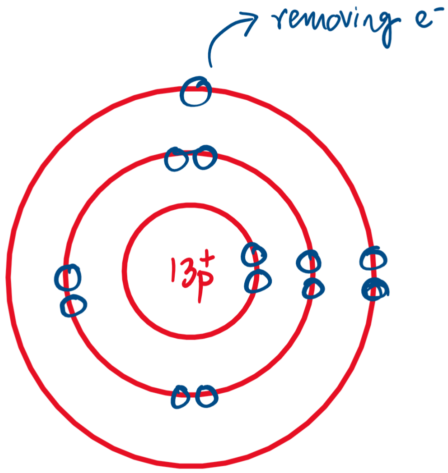
$Al^{1+}_{(g)} \longrightarrow Al^{3+}_{(g)} + 2e$ 2nd + 3rd I.E

1st Ionization Energy

Energy needed to remove 1 mol of e- from 1 mol of gaseous atoms to form 1 mol of gaseous +1 ions

2nd Ionization Energy

Energy needed to remove 1 mol of e- from 1 mol of gaseous +1 ions to form 1 mol of gaseous +2 ions

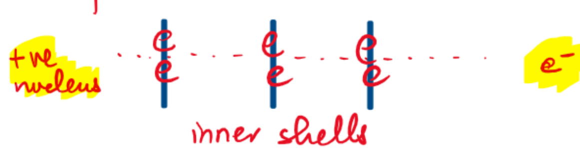


factors (Ionization Energy)

1. proton no. / nuclear charge
   - more protons ⟶ more attraction for e⁻, higher I.E

2. distance b/w e⁻ and nucleus / atomic or ionic radius
   - more distance ⟶ easy to remove e⁻, lower I.E

3. shielding / no of inner shells



   because of inner shells, attraction b/w e⁻ and nucleus decreases,
   - lower I.E

4. net +ve charge on ion

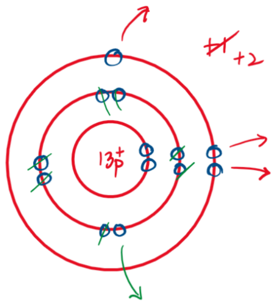
$$Na^{+} \longrightarrow Na^{+2} + e$$

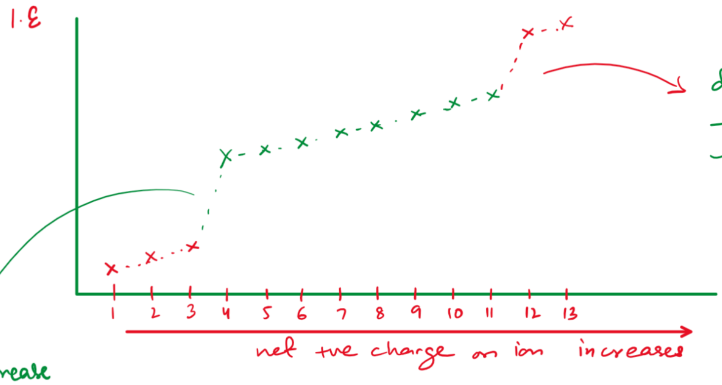
$$Na^{+7} \longrightarrow Na^{+8} + e$$

   greater net +ve charge, more difficult to remove e⁻
   higher 1st I.E

5. subshells (not important)
   only to be discussed in specific cases

Successive Ionization Energy



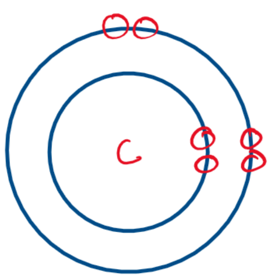


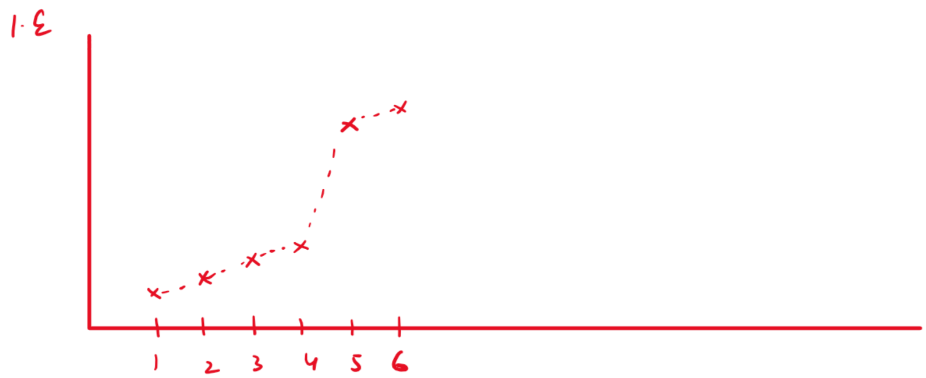
drastic increase
- less distance
- less shielding

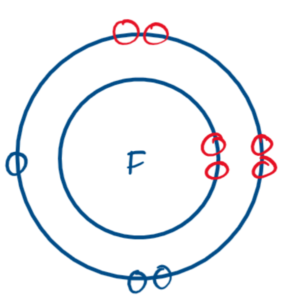
drastic increase
- less distance
- less shielding

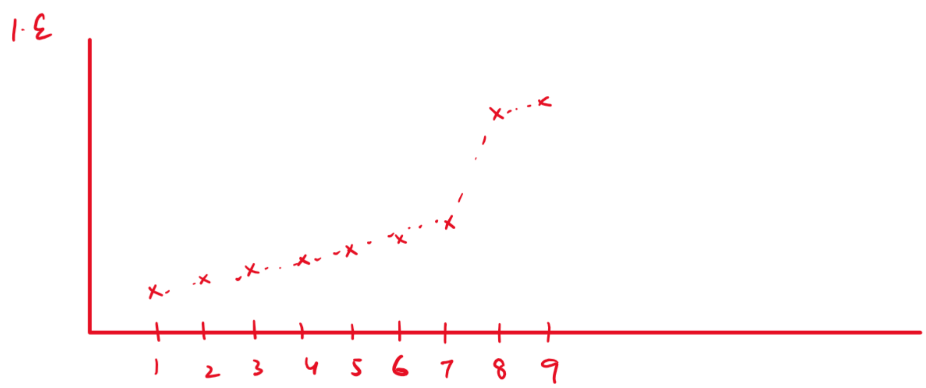
* no of e^- in outershell
* no of shells

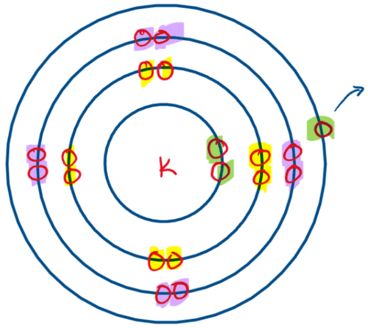
Group No
(Properties)

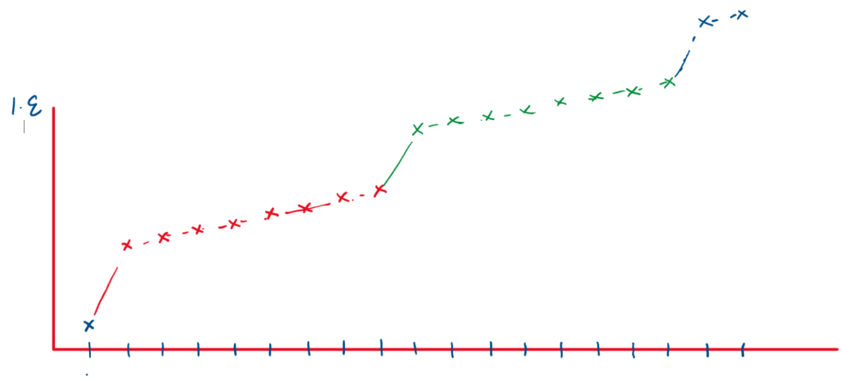




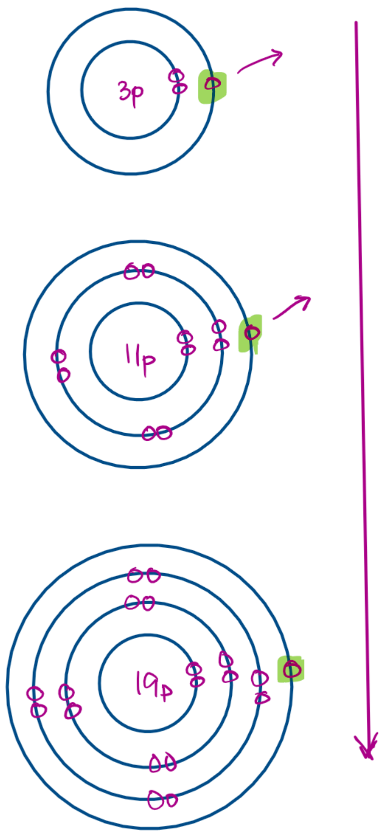






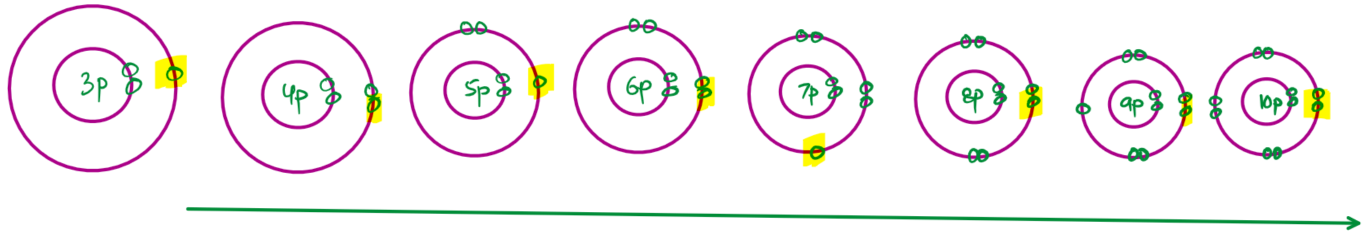


1st Ionization Energy down the group



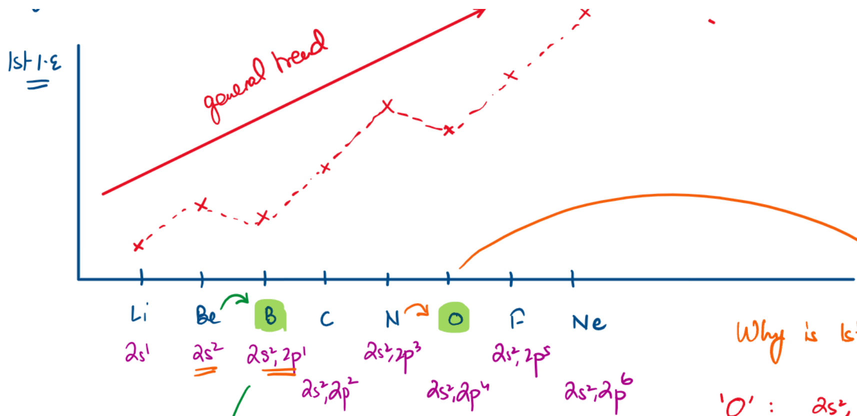
down the group, 1st I.E decreases
- atomic radius and shielding increases
attraction b/w nucleus and valence e⁻ decreases
despite the fact that nuclear charge increases

1st I.E across the Period



- nuclear charge increases
- same shielding.
- distance slightly decreases (more protons, more attraction for e-)

→ attraction b/w nucleus and valence e⁻ increases
higher 1st I.E



Why is ionization of B less than Be

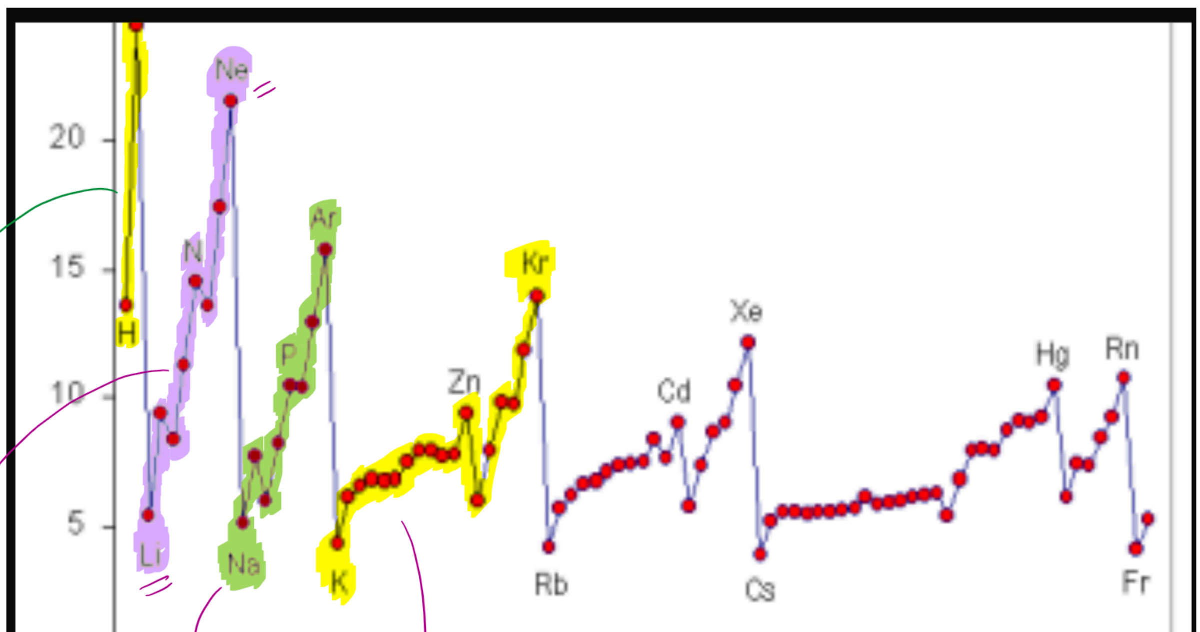
In B, e^- is removed from a higher energy p subshell, which is more shielded and further away compared to 2s subshell in Be

Why is 1st I.E of 'O' less than N

'O' : $2s^2, 2p^4$ $2p_x^2, 2p_y^1, 2p_z^1$

'N' : $2s^2, 2p^3$ $2p_x^1, 2p_y^1, 2p_z^1$

In O e^- is removed from a paired p subshell and electron - electron repulsion (spin-pair repulsion) it is easier to remove e^- in O compared to N where e^- were removed from unpaired p subshell



1st period

2nd Period.

3rd Period

4th Period
has 10 extra transition metals
invariant ionization

$_{26}Fe$ $1s^2 \ldots 3d^6, 4s^2$

$_{28}Ni$ $1s^2 \ldots 3d^8, 4s^2$

more protons, stronger attraction
shielding increases, e^- are always added to inner shells, weaker attraction

cancel each other