Periodic Classification of elements

- Dobereiner’s Triads
- Newlands’ Law of Octaves
- Mendeleev’s Periodic Table
- Modern Periodic Table

Dobereiner’s Triads

- Tried to arrange elements in group of 3- called Triads
- the atomic mass of the middle element was roughly the average of the atomic masses of the other two elements.
- Li- 6.3, Na-23, K- 39

<u>Limitation</u>

Only 3 triads identified

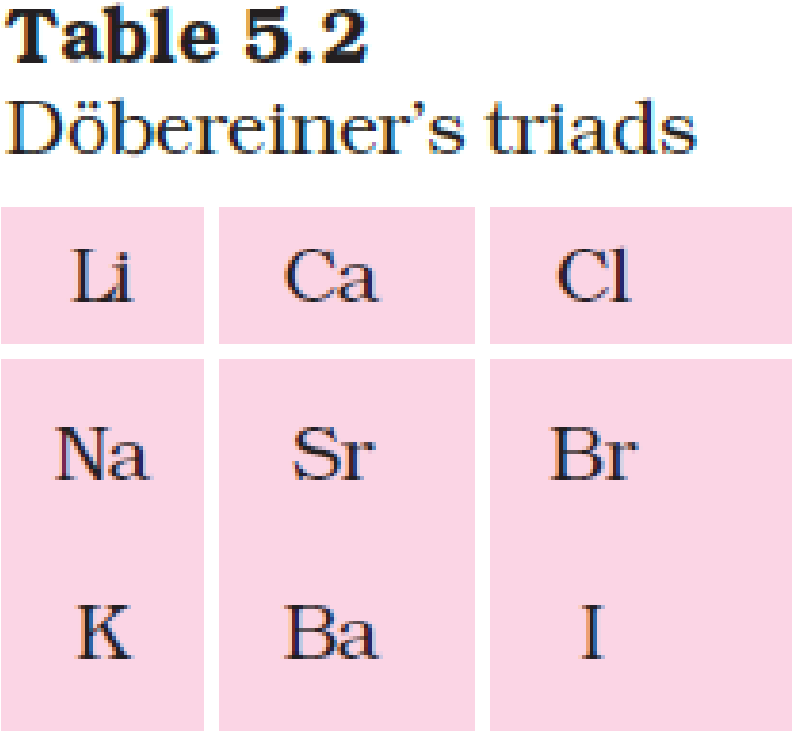


Table 5.2

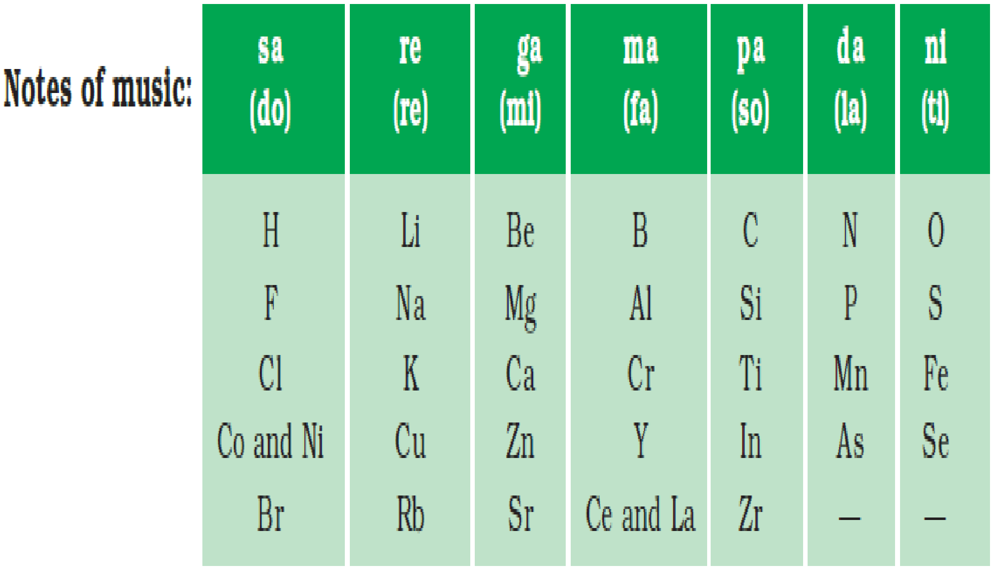
Döbereiner’s triads

Li	Ca	Cl
Na	Sr	Br
K	Ba	I

Newlands Law of Octaves

- In 1866, John Newlands arranged the then known elements in the order of increasing atomic masses
- Started with hydrogen (1) and ended with thorium (56)
- Every 8th element had similar property as first

Table 5.3 Newlands' Octaves



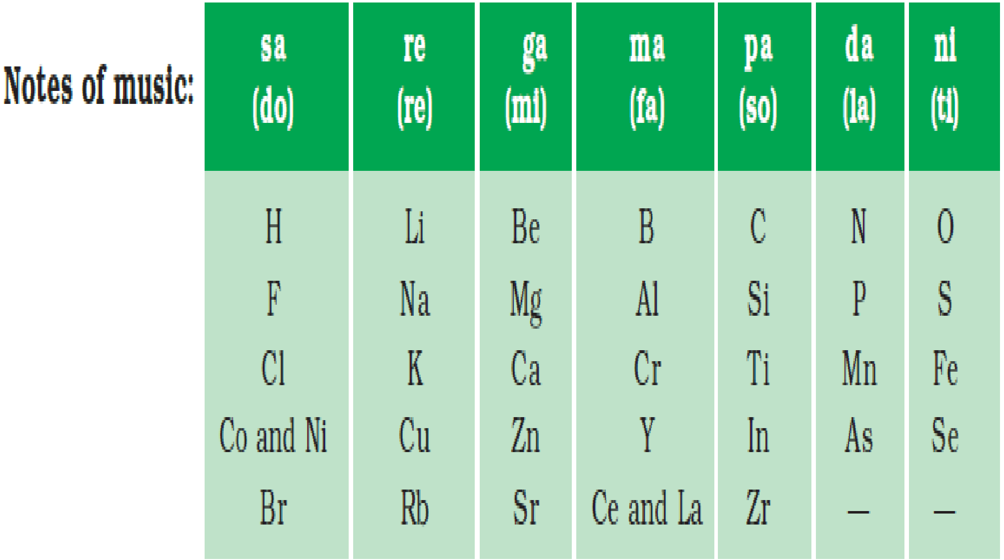
Notes of music:	sa (do)	re (re)	ga (mi)	ma (fa)	pa (so)	da (la)	ni (ti)
	H	Li	Be	B	C	N	O
	F	Na	Mg	Al	Si	P	S
	Cl	K	Ca	Cr	Ti	Mn	Fe
	Co and Ni	Cu	Zn	Y	In	As	Se
	Br	Rb	Sr	Ce and La	Zr	–	–

Newlands Law of Octaves-Limitations

Some Unlike elements under the same note

Ex: cl and co. Co more like fe, which is at far end of table

Table 5.3 Newlands' Octaves



Notes of music:	sa (do)	re (re)	ga (mi)	ma (fa)	pa (so)	da (la)	ni (ti)
	H	Li	Be	B	C	N	O
	F	Na	Mg	Al	Si	P	S
	Cl	K	Ca	Cr	Ti	Mn	Fe
	Co and Ni	Cu	Zn	Y	In	As	Se
	Br	Rb	Sr	Ce and La	Zr	—	—

Mendeleev’s Periodic Table

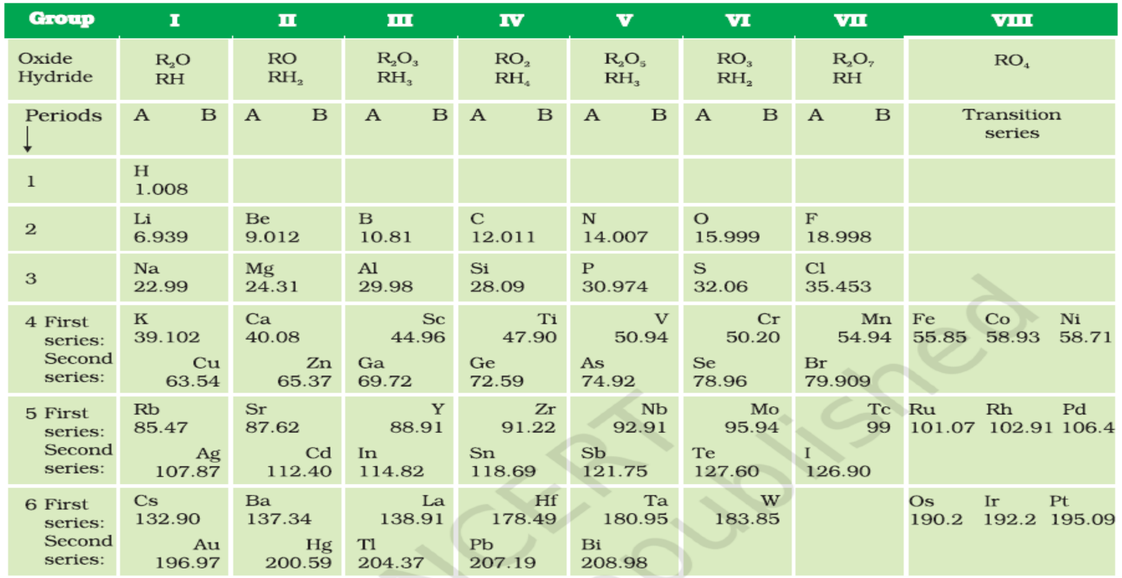
- Elements arranged based on

1. Fundamental property- Atomic Mass
2. Similarity of the Chemical Properties

- Chemical Property determined based on formation of compounds on reacting with oxygen and hydrogen- 2 most reactive elements

MENDELEEV PERIODIC TABLE

Table 5.4 Mendeléev's Periodic Table



Group	I	II	III	IV	V	VI	VII	VIII
Oxide Hydride	R_2O RH	RO RH_2	R_2O_3 RH_3	RO_2 RH_4	R_2O_5 RH_3	RO_3 RH_2	R_2O_7 RH	RO_4
Periods ↓	A B	A B	A B	A B	A B	A B	A B	Transition series
1	H 1.008							
2	Li 6.939	Be 9.012	B 10.81	C 12.011	N 14.007	O 15.999	F 18.998	
3	Na 22.99	Mg 24.31	Al 29.98	Si 28.09	P 30.974	S 32.06	Cl 35.453	
4 First series: Second series:	K 39.102 Cu 63.54	Ca 40.08 Zn 65.37	Sc 44.96 Ga 69.72	Ti 47.90 Ge 72.59	V 50.94 As 74.92	Cr 50.20 Se 78.96	Mn 54.94 Br 79.909	Fe 55.85 Co 58.93 Ni 58.71
5 First series: Second series:	Rb 85.47 Ag 107.87	Sr 87.62 Cd 112.40	Y 88.91 In 114.82	Zr 91.22 Sn 118.69	Nb 92.91 Sb 121.75	Mo 95.94 Te 127.60	Tc 99 I 126.90	Ru 101.07 Rh 102.91 Pd 106.4
6 First series: Second series:	Cs 132.90 Au 196.97	Ba 137.34 Hg 200.59	La 138.91 Tl 204.37	Hf 178.49 Pb 207.19	Ta 180.95 Bi 208.98	W 183.85		Os 190.2 Ir 192.2 Pt 195.09

Vertical: Group

Horizontal: period

Anamoly: Co and Ni

Achievements of Mendeleev Periodic Table

- Predicted the existence of some elements by leaving gaps in periodic table
- Gave a prefix Eka to such elements in the same group
- When Noble gases were discovered, they could be placed undisturbed in a new group

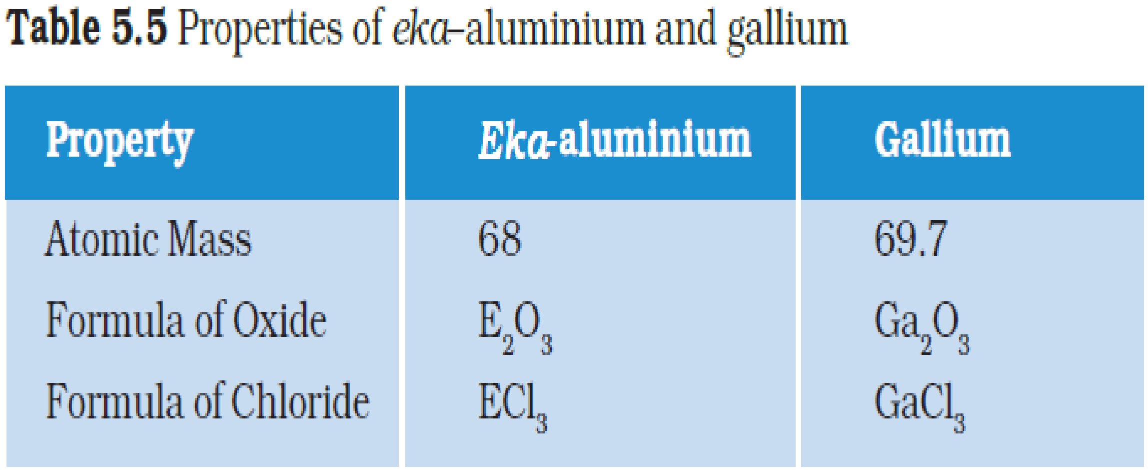


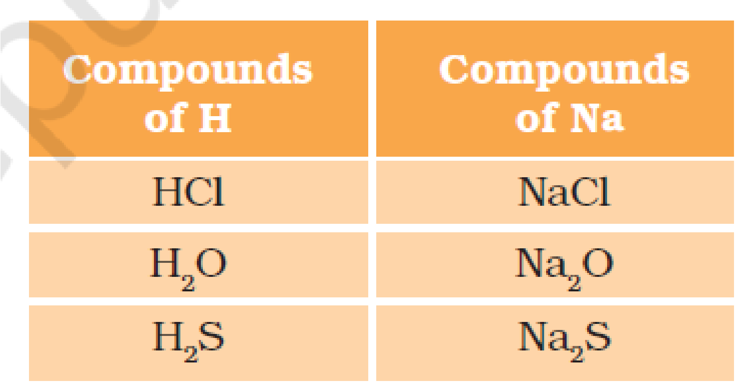
Table 5.5 Properties of *eka*–aluminium and gallium

Property	***Eka*-aluminium**	**Gallium**
Atomic Mass	68	69.7
Formula of Oxide	E_2O_3	Ga_2O_3
Formula of Chloride	ECl_3	$GaCl_3$

Mendeleev table-Limitations

1. No fixed position for Hydrogen. This was due to isotopes being discovered long after Mendeleev periodic table.

2. Atomic masses do not increase in a regular manner. Hence not possible to predict how many element could be discovered between 2 elements



Compounds of H	Compounds of Na
HCl	NaCl
H_2O	Na_2O
H_2S	Na_2S

Modern periodic Table- Henry Moseley

1. Moseley showed that atomic number is more of fundamental property than atomic mass
2. Elements arranged based on increasing atomic number
3. Due to this arrangement, prediction of new elements were more precise
4. Anomalies of Mendeleev table resolved

MODERN PERIODIC TABLE

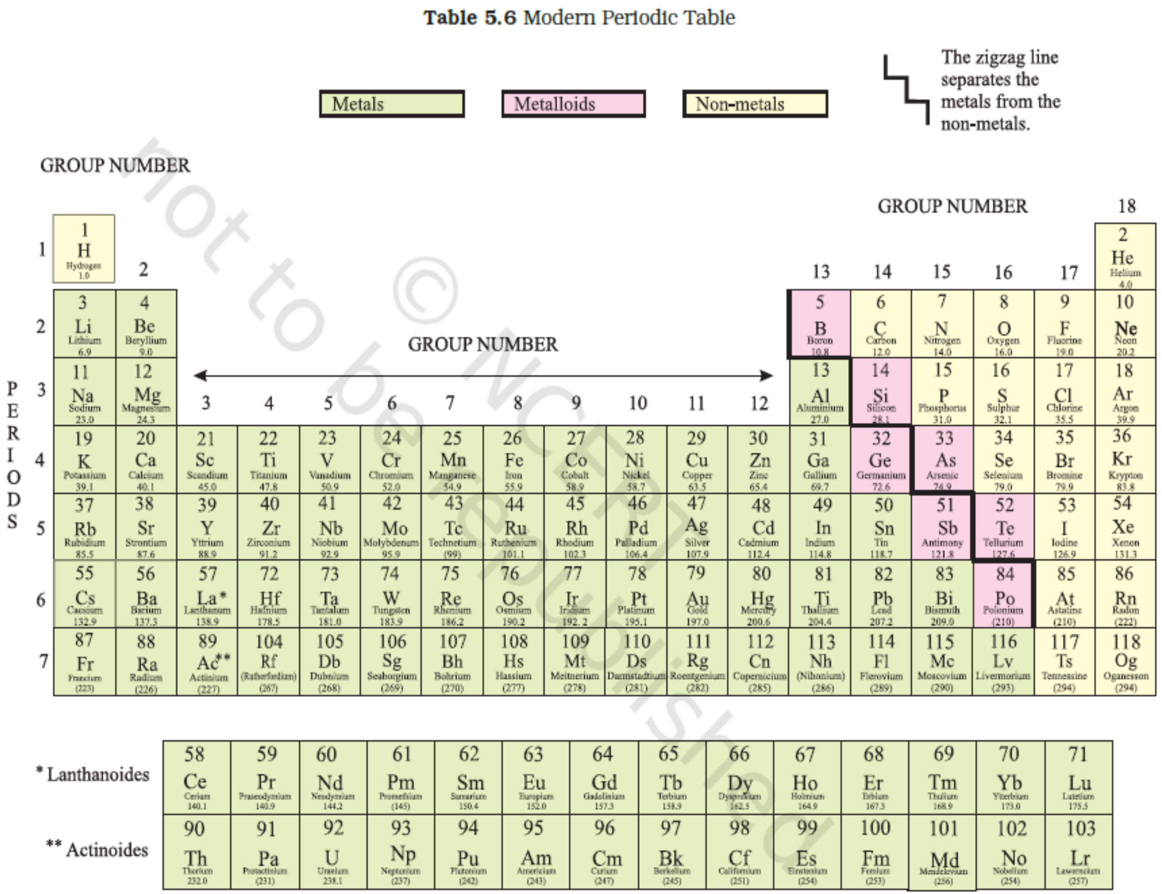


Table 5.6 Modern Periodic Table

Metals

Metalloids

Non-metals

The zigzag line separates the metals from the non-metals.

PERIODS	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	1 H Hydrogen 1.0																	2 He Helium 4.0
2	3 Li Lithium 6.9	4 Be Beryllium 9.0											5 B Boron 10.8	6 C Carbon 12.0	7 N Nitrogen 14.0	8 O Oxygen 16.0	9 F Fluorine 19.0	10 Ne Neon 20.2
3	11 Na Sodium 23.0	12 Mg Magnesium 24.3											13 Al Aluminium 27.0	14 Si Silicon 28.1	15 P Phosphorus 31.0	16 S Sulphur 32.1	17 Cl Chlorine 35.5	18 Ar Argon 39.9
4	19 K Potassium 39.1	20 Ca Calcium 40.1	21 Sc Scandium 45.0	22 Ti Titanium 47.8	23 V Vanadium 50.9	24 Cr Chromium 52.0	25 Mn Manganese 54.9	26 Fe Iron 55.9	27 Co Cobalt 58.9	28 Ni Nickel 58.7	29 Cu Copper 63.5	30 Zn Zinc 65.4	31 Ga Gallium 69.7	32 Ge Germanium 72.6	33 As Arsenic 74.9	34 Se Selenium 79.0	35 Br Bromine 79.9	36 Kr Krypton 83.8
5	37 Rb Rubidium 85.5	38 Sr Strontium 87.6	39 Y Yttrium 88.9	40 Zr Zirconium 91.2	41 Nb Niobium 92.9	42 Mo Molybdenum 95.9	43 Tc Technetium (99)	44 Ru Ruthenium 101.1	45 Rh Rhodium 102.3	46 Pd Palladium 106.4	47 Ag Silver 107.9	48 Cd Cadmium 112.4	49 In Indium 114.8	50 Sn Tin 118.7	51 Sb Antimony 121.8	52 Te Tellurium 127.6	53 I Iodine 126.9	54 Xe Xenon 131.3
6	55 Cs Caesium 132.9	56 Ba Barium 137.3	57 La* Lanthanum 138.9	72 Hf Hafnium 178.5	73 Ta Tantalum 181.0	74 W Tungsten 183.9	75 Re Rhenium 186.2	76 Os Osmium 190.2	77 Ir Iridium 192. 2	78 Pt Platinum 195.1	79 Au Gold 197.0	80 Hg Mercury 200.6	81 Ti Thallium 204.4	82 Pb Lead 207.2	83 Bi Bismuth 209.0	84 Po Polonium (210)	85 At Astatine (210)	86 Rn Radon (222)
7	87 Fr Francium (223)	88 Ra Radium (226)	89 Ac** Actinium (227)	104 Rf (Rutherfordium) (267)	105 Db Dubnium (268)	106 Sg Seaborgium (269)	107 Bh Bohrium (270)	108 Hs Hassium (277)	109 Mt Meitnerium (278)	110 Ds Darmstadtium (281)	111 Rg Roentgenium (282)	112 Cn Copernicium (285)	113 Nh (Nihonium) (286)	114 Fl Flerovium (289)	115 Mc Moscovium (290)	116 Lv Livermorium (293)	117 Ts Tennessine (294)	118 Og Oganesson (294)

* Lanthanoides	58 Ce Cerium 140.1	59 Pr Praseodymium 140.9	60 Nd Neodymium 144.2	61 Pm Promethium (145)	62 Sm Samarium 150.4	63 Eu Europium 152.0	64 Gd Gadolinium 157.3	65 Tb Terbium 158.9	66 Dy Dysprosium 162.5	67 Ho Holmium 164.9	68 Er Erbium 167.3	69 Tm Thulium 168.9	70 Yb Ytterbium 173.0	71 Lu Lutetium 175.5
** Actinoides	90 Th Thorium 232.0	91 Pa Protactinium (231)	92 U Uranium 238.1	93 Np Neptunium (237)	94 Pu Plutonium (242)	95 Am Americium (243)	96 Cm Curium (247)	97 Bk Berkelium (245)	98 Cf Californium (251)	99 Es Einstenium (254)	100 Fm Femium (253)	101 Md Mendelevium (256)	102 No Nobelium (254)	103 Lr Lawrencium (257)

Filling up of electron Shells-Principal Quantum Number (n)

- Closest shell to nucleus is K shell, next L, M and so on
- Principal Quantum numbers are n= 1,2,3, 4 etc
- Each shell holds 2n2 Electrons
- K- 2 electrons
- L - 8 electrons
- M -18 Electrons
- N - 32 Electrons

Electron Sub Shells- Azimuthal Quantum Number (l)

- In each shell, electrons exist in sub-energy levels or sub-shells.
- Azimuthal Quantum number defines the sub shells, having values from 0 to n-1, as follows
- If n=1, l=0 (Only 1 value->1 level -> s)
- If n=2, l=0,1 (2 values->2 levels->s,p)
- If n=3, l=0,1,2 (3 values->3 levels->s,p,d)
- If n=4, l=0,1,2,3 (4 values->4 levels->s,p,d,f)

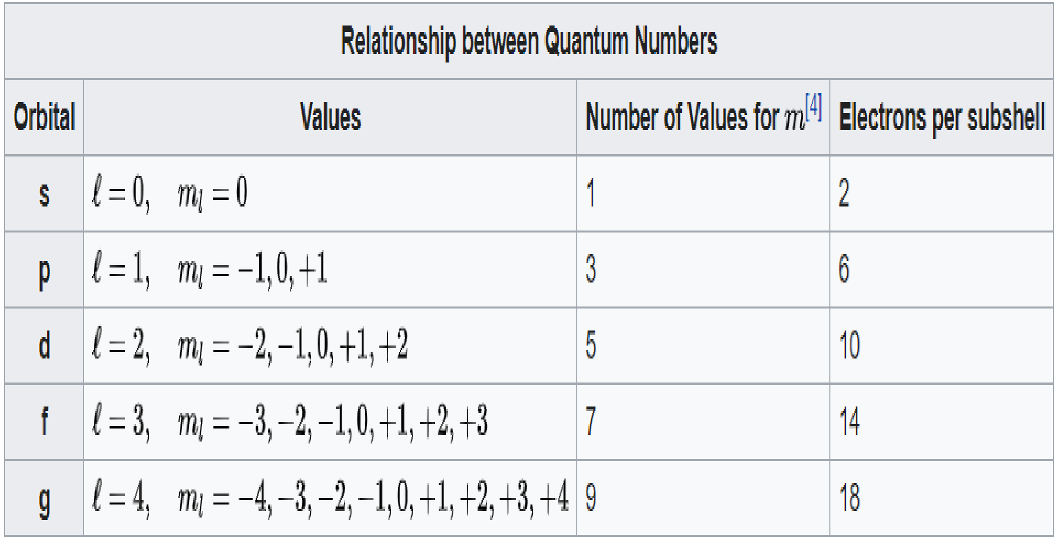
Electron Sub Shells- Azimuthal Quantum Number (l)

- The sub shells are named s,p,d and f. Maximum electrons in each sub shell is as follows (Given by 4l+2)
- s - 2 electrons
- p- 6 electrons
- d-10 Electrons
- f- 14 Electrons

Azimuthal Quantum number l for sub-shells are: s=0, p=1,d=2 and f=3

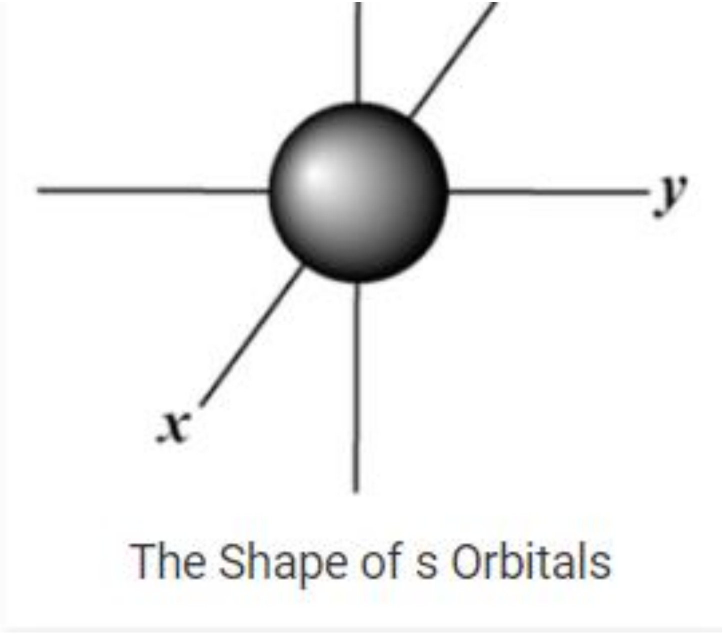
Orbitals in Sub Shells- Magnetic Quantum Number (m)

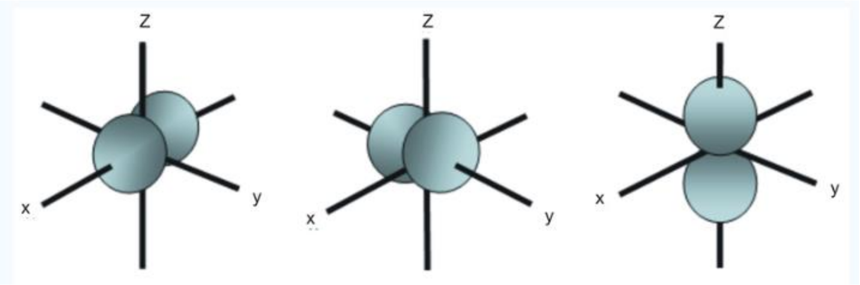
- In a strong magnetic field, the sub-shells are resolved into different orientations denoted by magnetic quantum number m
- This value depends on l. where m=-l through 0 to +l



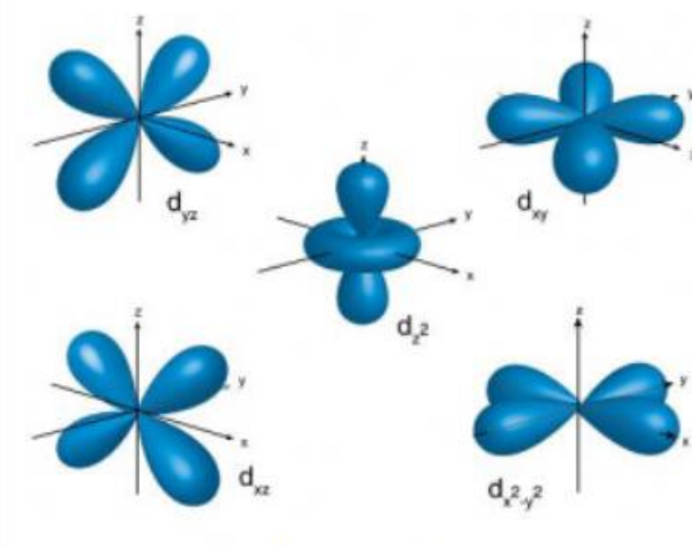
Relationship between Quantum Numbers

Orbital	Values	Number of Values for m[4]	Electrons per subshell
s	$\ell = 0, \quad m_l = 0$	1	2
p	$\ell = 1, \quad m_l = -1, 0, +1$	3	6
d	$\ell = 2, \quad m_l = -2, -1, 0, +1, +2$	5	10
f	$\ell = 3, \quad m_l = -3, -2, -1, 0, +1, +2, +3$	7	14
g	$\ell = 4, \quad m_l = -4, -3, -2, -1, 0, +1, +2, +3, +4$	9	18

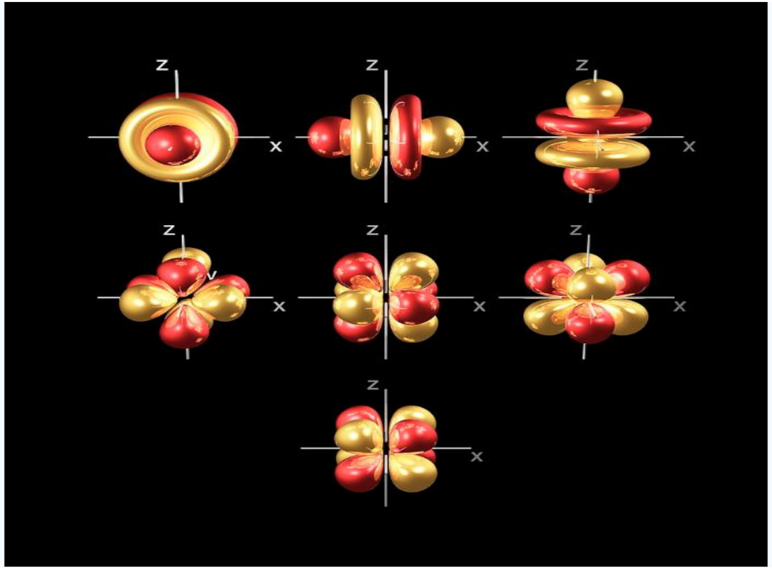




Shapes of the orbitals based on Azimuthal Quantum Number- S & P



The Shape of d Orbitals



Shapes of the orbitals based on Azimuthal Quantum Number- d & f

Spin Quantum Number (s)

- The electron in the atom rotates not only around the nucleus but also around its own axis and two opposite directions of rotation are possible (clock wise and anticlock wise).
- Therefore the spin quantum number can have only two values +1/2 or –1/2.

Pauli’s exclusion principle

“it is impossible for any two electrons in a given atom to have all the four quantum numbers identical” i.e., in an atom, two electrons can have maximum three quantum numbers (n, *l* and m) the same and the fourth(*s*) will definitely be having a different value.

Thus if s = +1/2 for one electron, s should be equal to –1/2 for the other electron. In other words the two electrons in the same orbital should have opposite spins (¯).

Use of Pauli's principle

The greatest use of the principle is that it is helpful in determining the maximum number of electrons that a main energy level can have.

- Let us illustrate this point by considering K and L shells
- (a) K-shell: For this shell n = 1. For n = 1, *l* = 0 and m = 0. Hence *s* can have a value either +1/2 or –1/2. The different values of n, *l*, m and s given above give the following two combinations of the four quantum numbers, keeping in view the exclusion principle.
- Combination (i) is for one electron and combination (ii) is for the other electron.
- (i) n = 1, *l* = 0, m = 0
- *s* = +1/2 (1st electron)
- (ii) n = 1, *l* = 0, m = 0,
- *s* = -1/2 (2nd electron)
- (Two electrons in *l* = 0 sub-shell i.e., 1*s*-orbital)
- These two combinations show that in K shell there is only one subshell corresponding to *l* = 0 value (*s*-sub-shell) contains only two electrons with opposite spins.

Use of Pauli's principle

The greatest use of the principle is that it is helpful in determining the maximum number of electrons that a main energy level can have.

- (b) L-shell: For this shell n = 2. For n = 2 the different values of *l*, m and *s* give the following eight combinations of four quantum numbers.
- (i) n= 2, *l* = 0, m = 0, *s* = +1/2
- (ii) n = 2, *l* = 0, m = 0, *s* = -1/2
- (iii) n = 2, *l* = 1, m = 0, *s* = +1/2
- (iv) n = 2, *l* = 1, m = 0, *s* = -1/2
- (v) n = 2, *l* = 1, m = +1, *s* = +1/2
- (vi) n = 2, *l* = 1, m = +1, *s* = -1/2
- (vii) n = 2, *l* = 1, m = -1, s = +1/2
- (viii) n = 2, *l* = 1, m = -1, s = -1/2
- Eight combinations given above show that L shell is divided into two sub-shells corresponding to *l* = 0 (*s* sub-shell) and *l* = 1 (p sub-shell) and this shell cannot contain more than 8 electrons, i.e., its maximum capacity for keeping the electrons is eight.

Aufbau principle

"In the ground state of the atoms, the orbitals are filled in order of their increasing energies" i.e., electrons first occupy the lowest-energy orbital available to them and enter into higher energy orbitals only after the lower energy orbitals are filled

The order in which the energies of the orbitals increase and hence the order in which the orbitals are filled is as follows: 1s, 2s, 2p, 3s, 3p, 4s, 3d, 4p, 5s, 4d, 5p, 6s, 4f, 5d, 6p, 7s……………

Aufbau principle

The states crossed by same red arrow have same $n + \ell$ value. The direction of the red arrow indicates the order of state filling.

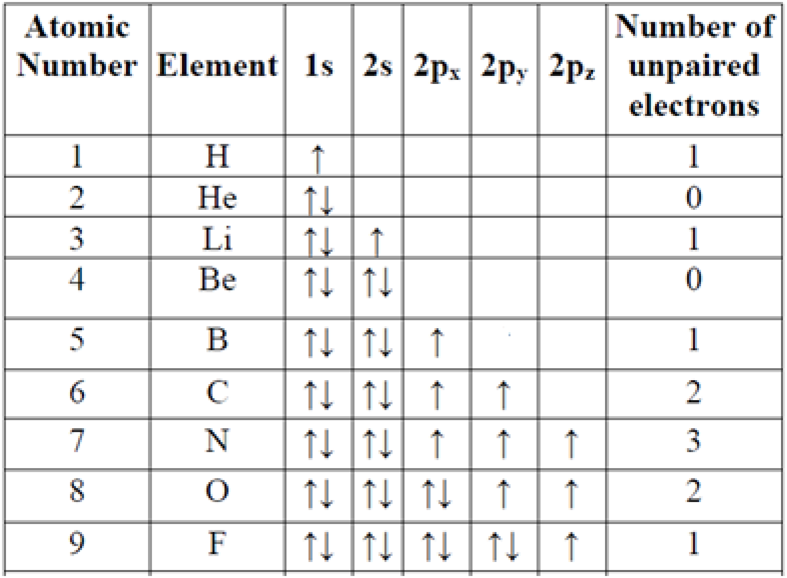
Hund’s Rule of maximum multiplicity

“Hund’s rule of maximum multiplicity states, that in filling p, d or f orbitals, as many unpaired electrons as possible are placed before pairing of electrons with opposite spin is allowed”

Pairing of electrons requires energy. Therefore no pairing occurs until all orbitals of a given sublevel are half filled. This is known as Hund’s rule of maximum multiplicity

Hund's rule of maximum multiplicity

- Thus, if three electrons are to be filled in the p- level of any shell, one each will go into each of the three (*px, py, pz*) orbitals.
- The fourth electron entering the p-level will go to px orbital which now will have two electrons with opposite spins (as shown in pic) and said to be paired. The unpaired electrons play an important part in the formation of bonds.



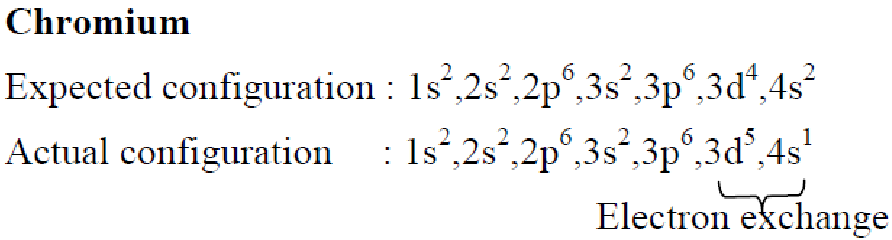
Atomic Number	**Element**	**1s**	**2s**	**$2p_x$**	**$2p_y$**	**$2p_z$**	**Number of unpaired electrons**
1	H	↑					1
2	He	↑↓					0
3	Li	↑↓	↑				1
4	Be	↑↓	↑↓				0
5	B	↑↓	↑↓	↑			1
6	C	↑↓	↑↓	↑	↑		2
7	N	↑↓	↑↓	↑	↑	↑	3
8	O	↑↓	↑↓	↑↓	↑	↑	2
9	F	↑↓	↑↓	↑↓	↑↓	↑	1

Stability of orbitals

- As per Hund's rule- Half filled or completely filled orbitals are stable
- The half-filled and completely filled electron configurations have symmetrical distribution of electrons and this symmetry leads to stability
- Thus the *p3,p6,d5,d10,f7* and *f14* configuration which are either completely filled or exactly half-filled are more stable.
- Moreover, in such configuration electron can exchange their positions among themselves to maximum extent

Filling up the orbitals and Hund’s rule illustration

- Chromium- Atomic Number 24
- K-2, L-8, N-2, M-12- Expected
- K-2, L-8, N-1, M-13- Actual

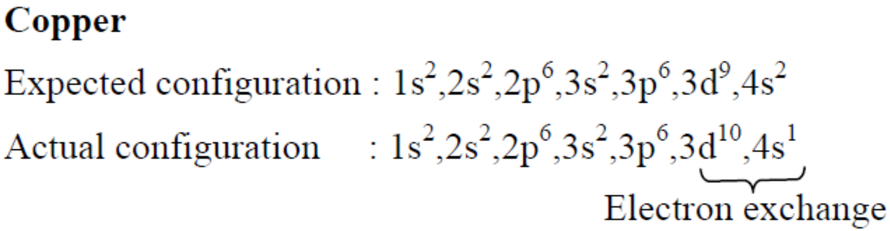


Chromium

Expected configuration : $1s^2,2s^2,2p^6,3s^2,3p^6,3d^4,4s^2$

Actual configuration : $1s^2,2s^2,2p^6,3s^2,3p^6,\underbrace{3d^5,4s^1}_{\text{Electron exchange}}$

- Copper- Atomic Number 29
- K-2, L-8, N-2, M-17- Expected
- K-2, L-8, N-2, M-17- Actual



Copper

Expected configuration : $1s^2,2s^2,2p^6,3s^2,3p^6,3d^9,4s^2$

Actual configuration : $1s^2,2s^2,2p^6,3s^2,3p^6,\underbrace{3d^{10},4s^1}_{\text{Electron exchange}}$