QUOTE

- **A MAN WOULD DO NOTHING, IF HE WAITED UNTIL HE COULD DO IT SO WELL THAT NO ONE WOULD FIND FAULT WITH WHAT HE HAS DONE**

---Cardinal Newman

ATOMIC STRUCTURE

In this topic we shall talk about:

(i) The atom and its constituents

(ii) The quantum Nos of the electron in an atom

(iii) Electronic Configuration of the elements

ATOMIC STRUCTURE

Define:

Atom is the basic unit of an element that can enter into (take part in a) chemical combination.

- **The Atom is made up of the Nucleus which is a dense central core within the Atom.**
- **The Nucleus is +vely charged**

➢ **SUB-ATOMIC PARTICLES**

- **Proton: +vely charged and located at the centre of the nucleus.**
- **Neutron: Electrically Neutral and also located at the nucleus.**

- Electron -vely charged

- The atom contains the same number of p as e; electrically neutral.

Particle	Mass (g)	Charge Unit
Electron	9.10938×10^{-28}	– 1
Proton	1.67262×10^{-24}	+1
Neutron	1.67262×10^{-24}	0

$$1 \text{ amu} = 1.66 \times 10^{-24} \text{ g.}$$

Note: Mass of the Proton is about 1840 times Mass of the electron

- **Atomic Number Z** → **No of p or e**
- **Atomic mass M** → **p + n**

Mass Number

$${}^{A}_{Z}\mathrm{X}$$

Atomic Number

e.g. $${}^{12}_{6}C$$

Mass Number = number of protons + number of Neutrons

= Atomic number + Number of Neutrons

The chemical properties of an element is determined by the electrons (electronic Conf.). i.e. by the electrons and NEVER by the Neutrons

ISOTOPES: Atoms that have the same Atomic number but different mass Numbers

$$^{235}_{92}U \qquad\qquad ^{238}_{92}U$$

Uranium two thirty-five **Uranium two thirty-eight**

$$^{1}_{1}H \qquad\qquad ^{2}_{1}H \qquad\qquad ^{3}_{1}H$$

Hydrogen **Deuterium** **Tritium**

Quantum Numbers

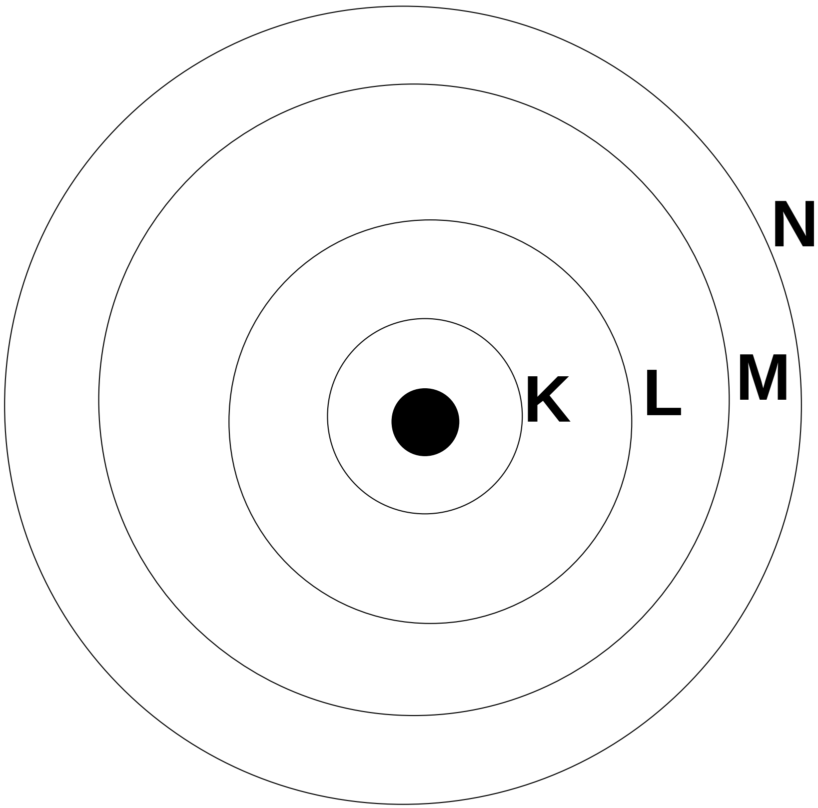
- **4 Quantum Numbers**
- **Principal Quantum No n:**
- **Takes values: n = 1, 2, 3, 4 etc.**
  - n ➔ **Specifies the energy of the electron**

$$E_n = -R_H\left(\frac{1}{n^2}\right)$$

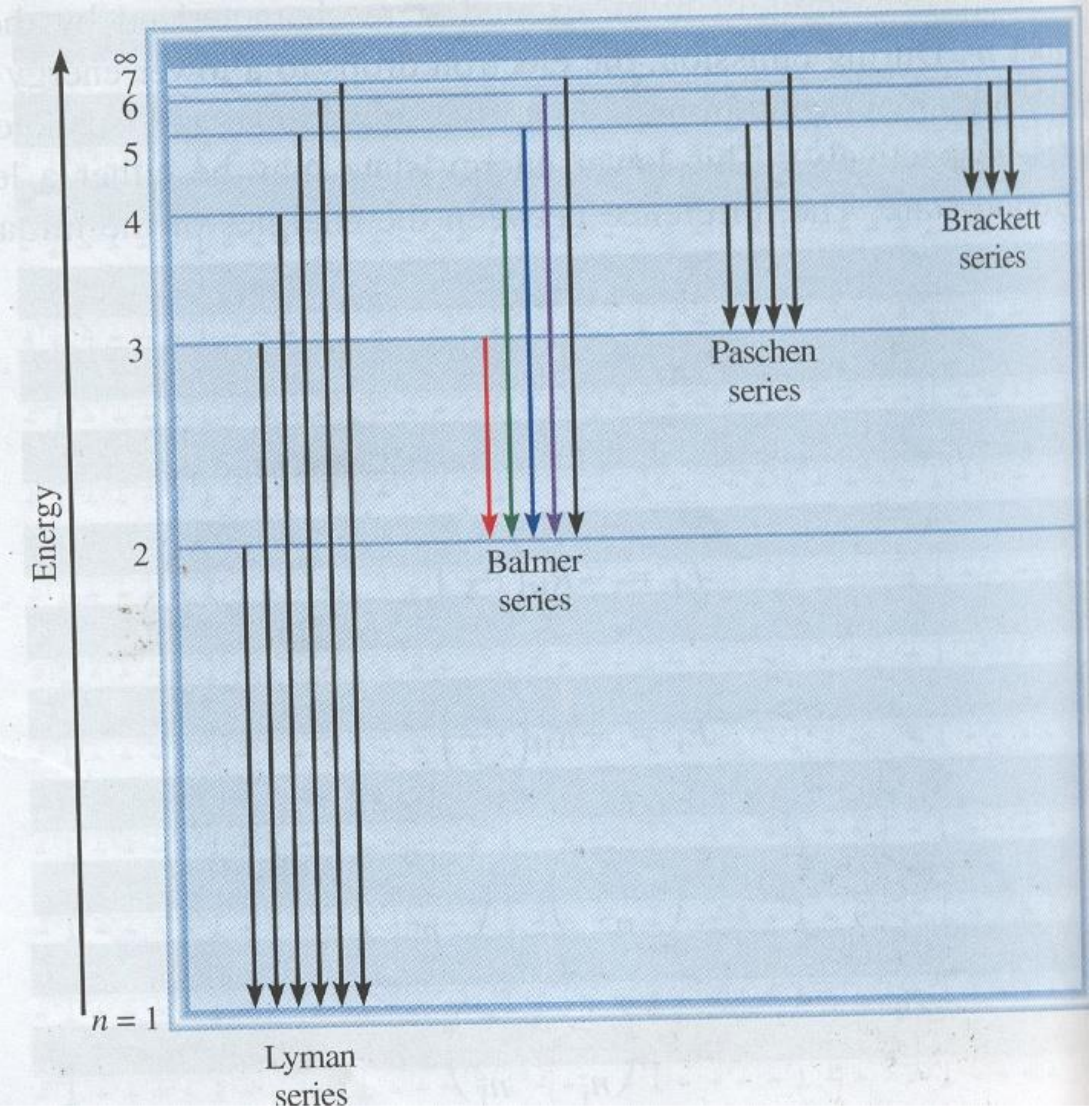
R_H **Is the Rydberg constant and has the value 2-18 x 10^{-18} J.**

The negative sign in the eq is an arbitrary convention, signifying that the energy of the electron in the atom is lower than the energy of a free electron, which is an election that is infinitely far from the nucleus. The energy of the free electron is arbitrarily assigned a value of zero. Mathematically, this corresponds to setting n equal to infinity in the eq. so that $E_{\infty} = 0$.

As the electron gets closer to the nucleus (as n decreases), E becomes larger in absolute value, but also more negative.



Shell	K	L	M	N	O
n	1	2	3	4	5



Energy
∞
7
6
5
4
3
2
n = 1
Lyman series
Balmer series
Paschen series
Brackett series

Suppose an electron is in an initial excited state n_i and during emission drops to a lower energy state n_f

The difference in energy between the two states is given by:

$$\Delta E = E_f - E_i$$

$$E_f = -R_H\left(\frac{1}{n_f^2}\right) \; and \; E_i = -R_H\left(\frac{1}{n_i^2}\right)$$

$$\Delta E = \left(\frac{-R_H}{n_f^2}\right) - \left(\frac{-R_H}{n_i^2}\right)$$

$$\Delta E = R_H\left(\frac{1}{n_i^2} - \frac{1}{n_f^2}\right)$$

Worked Example

Calculate the change in Energy in the transition of an electron from n_i = 5 to the n_f = 2 state in the hydrogen atom.

SOLUTION:

The energy change $\Delta E = E_f - E_i$

$$\Delta E = R_H\left(\frac{1}{n_i^2} - \frac{1}{n_f^2}\right)$$

$$= 2.18 \, x \, 10^{-18} J \left(\frac{1}{5^2} - \frac{1}{2^2}\right)$$

$$= - 4.58 \times 10^{-19} \text{ J}$$

Angular Momentum Quantum number, l

- **Angular Quantum number, l determines the shape of the orbital**

❖ Takes values from 0 to (n - 1)

Example:

When n = 1, then l = 0

n = 2, then l = 0, 1

n = 3, then l = 0, 1, 2

l	0	1	2	3	4	5
Name of Orbital	s	p	d	f	g	h

Where:

s stands for Sharp

p stands for Principal

d stands for Diffuse

f stands for Fundamental

These are spectroscopic terms. There are only 4 spectroscopic terms. After these the next orbital follow the alphabetic listing. The next orbital after f is the g orbital followed by h orbital as so forth.

Magnetic Quantum Number, m_l

m_l → Describes the orientation of the orbital in space.

Within a shell, the value of m depends on the value of the Angular momentum Quantum No l

- For a given value of l, there are (2l +1) integral values of m_l

Value : -l, (-l +1), …0, (+l – 1), +l

e.g. for l = 2

we have l = -2, -1, 0, +1, +2

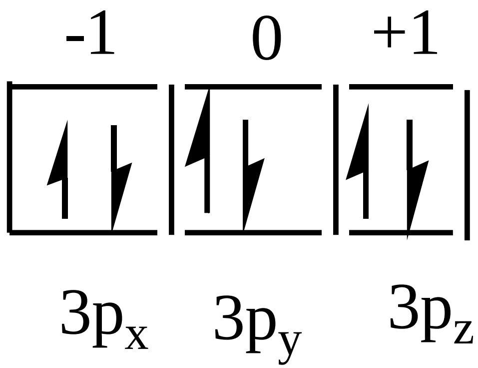
n	l	m_l	No of - Orbitals	Atomic Orbital Designations
1	0	0	1	1s
2	0 1	0 -1, 0, +1	1 3	2s $2p_x$, $2p_y$, $2p_z$
3	0 1 2	0 -1, 0, +1 -2, -1, 0, +1, +2	1 3 5	3s $3p_x$, $3p_y$, $3p_z$ $3d_{xy}$, $3d_{yz}$, $3d_{xz}$,

$3d_{x^2-y^2}$ $3d_{z^2}$

Spin quantum No

- m_s ➔Specifies the orientation of the electron's spin angular momentum
  - **Spin Quantum Number, m_s**
    - »**Value: ±½**

Write the Four quantum Numbers for six electrons in a 3p orbital.

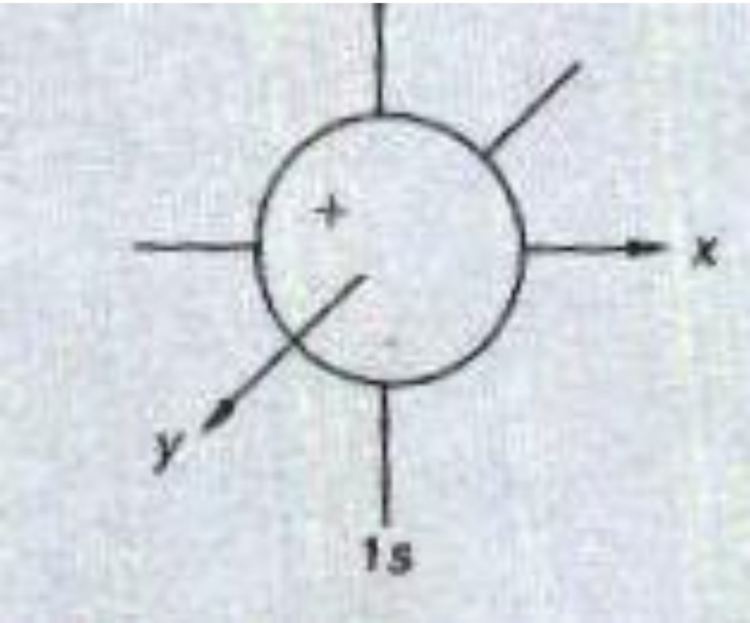


electron	n	l	m	s
1	3	1	-1	+½
2	3	1	0	+½
3	3	1	+1	+½
4	3	1	-1	-½
5	3	1	0	-½
6	3	1	+1	-½

SHAPE OF THE ORBITALS

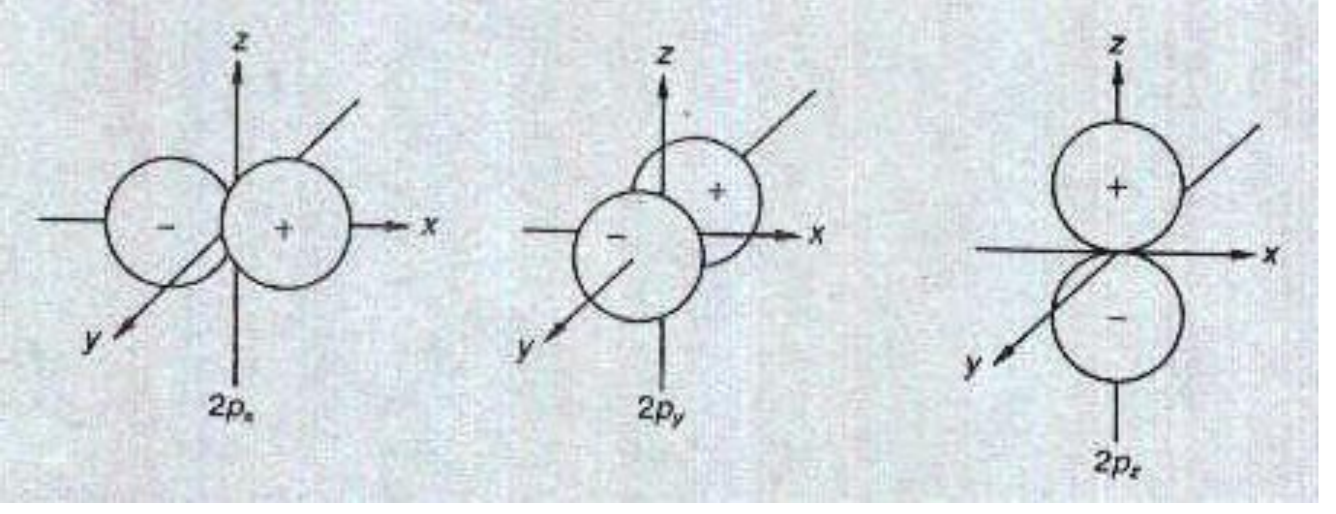
S-orbital:

Spherical in shape, centered at the nucleus.
Overlap equally well in all directions



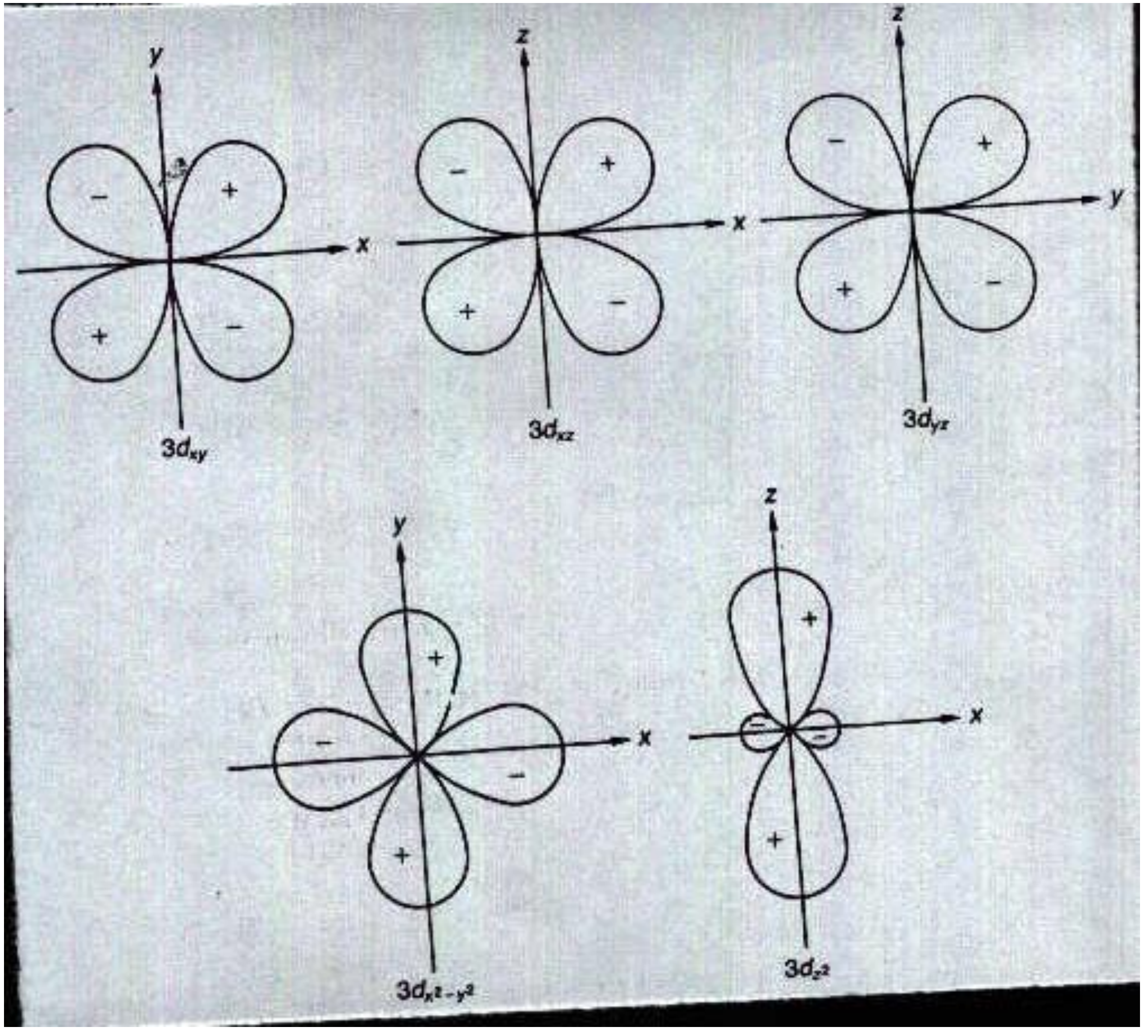
p-orbital:

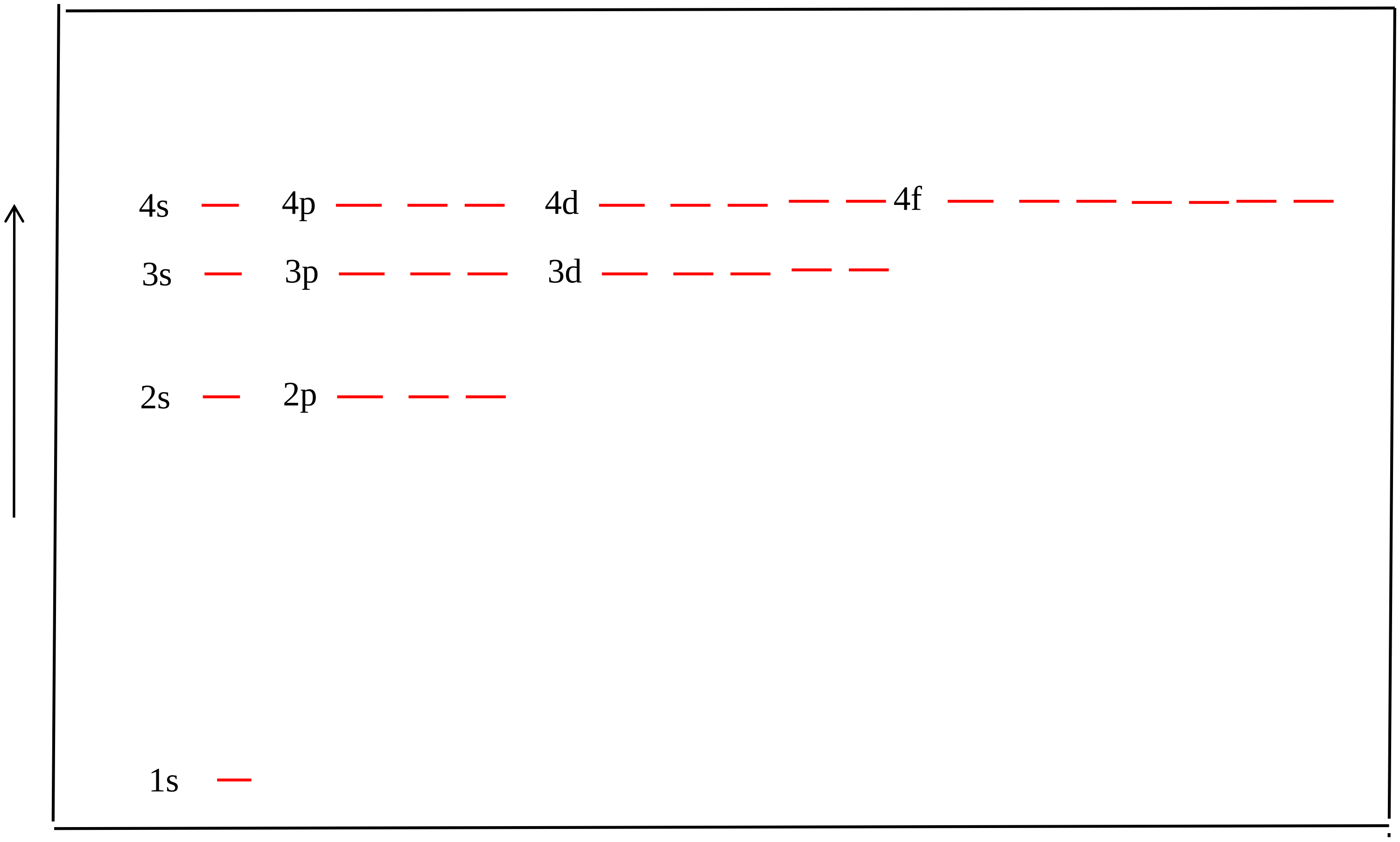
Dumb-belled shaped with two lopes directed along each of 3-axes



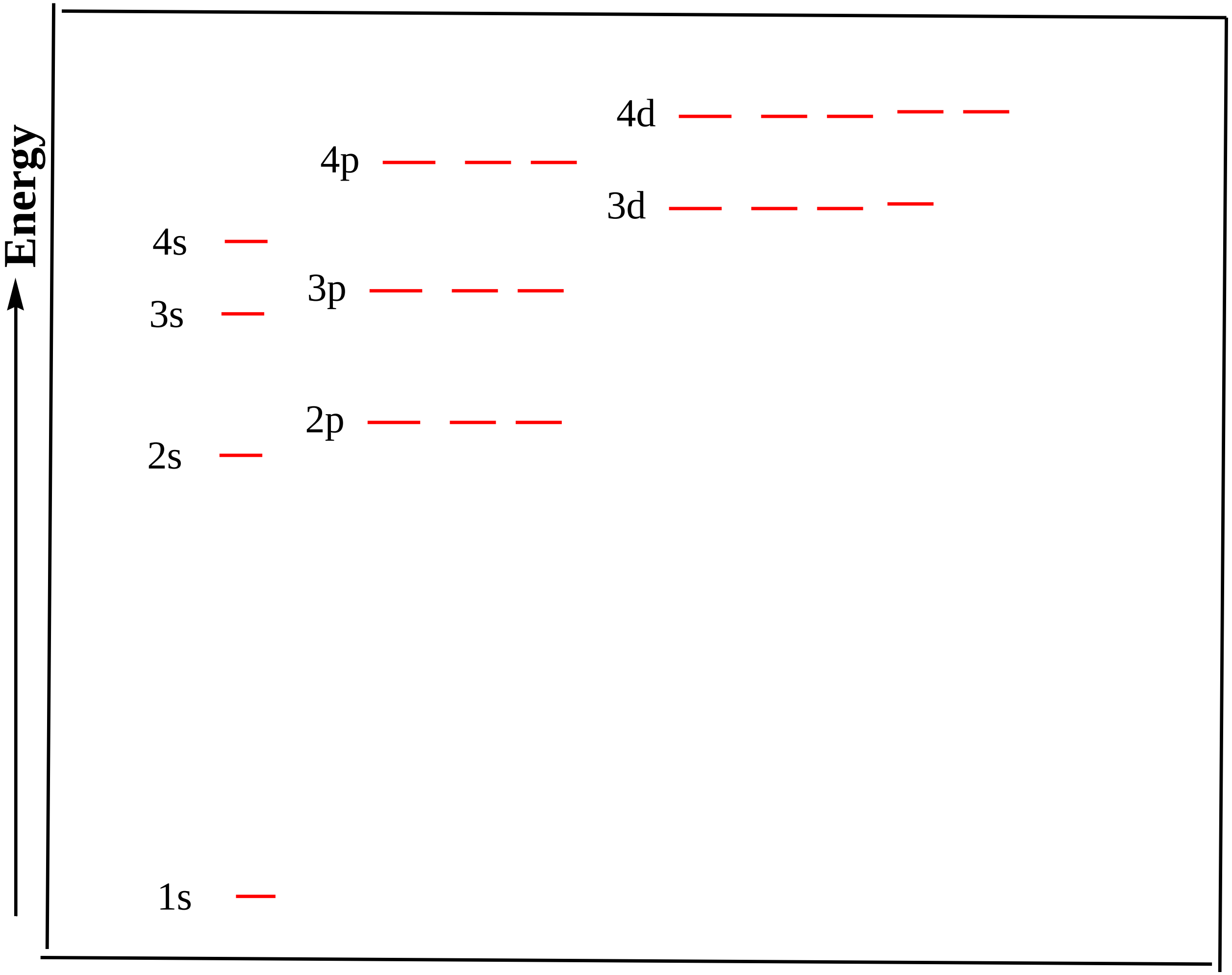
d-orbital

- Double dumb-bell shaped. **(5 d-orbitals)**



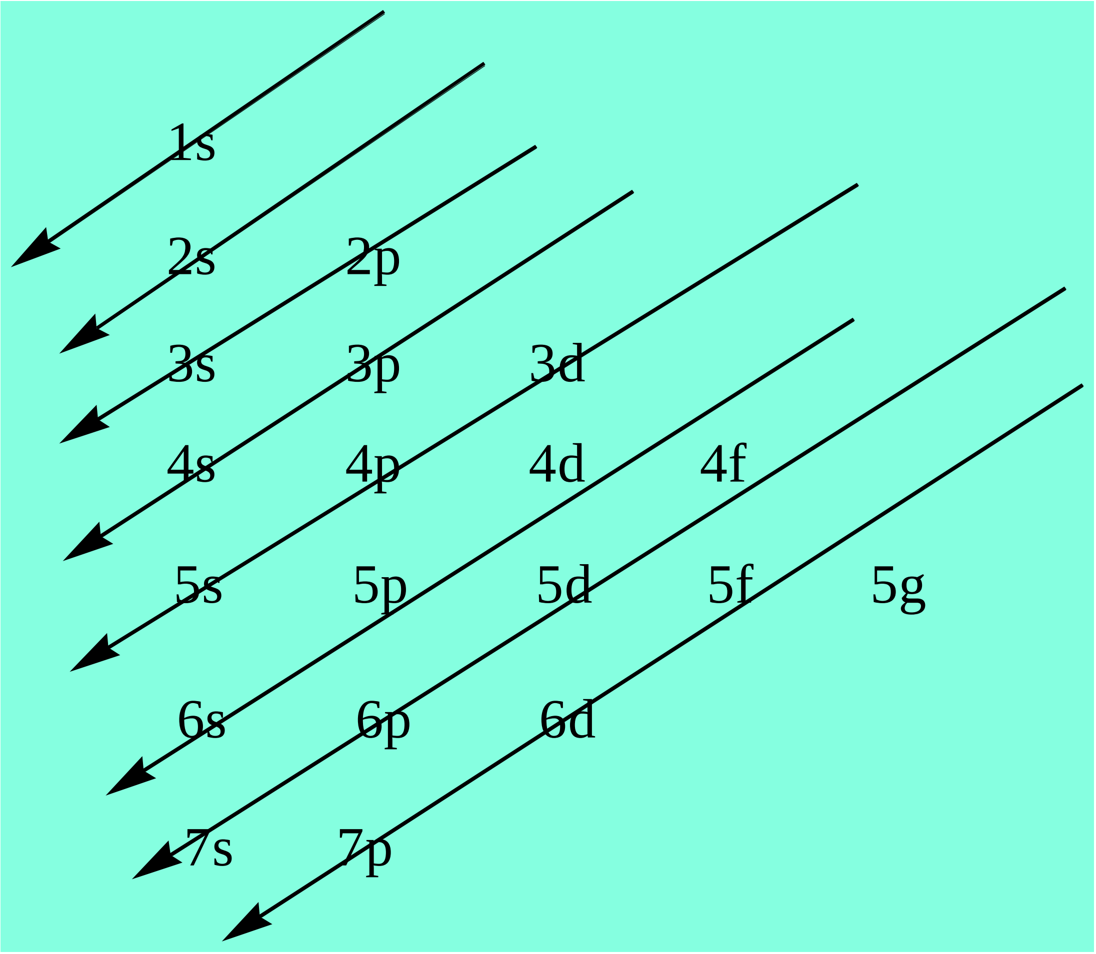


Orbital energy levels in the hydrogen atom



Orbital energy levels in a many-electron atom
Note that the energu depends on both n and l

Energies of the orbitals



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

n + l Rule

The order above follows what is known as the

(n + l) rule.

- The orbital with lowest value of n + l has the lowest energy.

- When two orbitals have the same value of n + l value, the one with the lower n value takes precedence in determining the lowest energy state.

- Examples: Which has the lowest energy: (a) (i) 4s or 4p; (ii) 5s and 4p.
- SOLUTION:
- (i) 4s = 4 + 0 = 4, 4p = 4 + 1 = 5. Therefore 4s has a lower energy.
- (ii) 5s = 5 + 0 = 5, 4p = 4 + 1 = 5. Since n value for 4p is lower, the 4p orbital has a lower energy.

FILLING OF THE ORBITALS

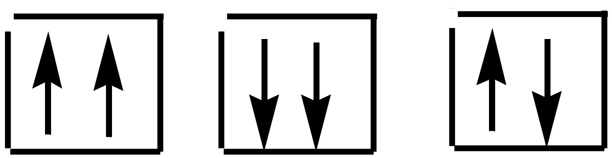
- **Aufau Principle (The filling Process)**

- **Electrons occupy orbital with lowest energy before filling those with higher energy.**

- **e.g. Fill 1s before the 2s. Similarly Fill the 2s before filling the 2p**

Pauli Exclusion Principle:

No two electrons in an atom can have the same set of four quantum numbers.

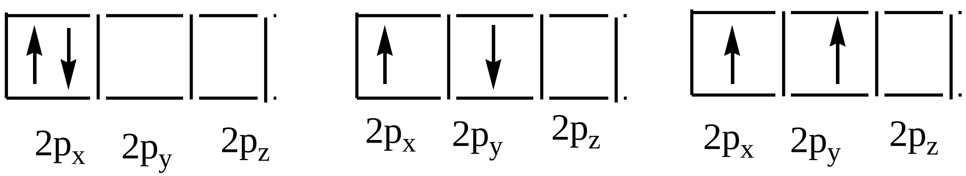


$1s^2$ $1s^2$ $1s^2$

Hund's Rule of maximum multiplicity.

The most stable arrangement of electrons in a subshell is the one with the greatest number of parallel spins (unpaired electrons).

Consider the electronic configuration of carbon $1s^2 2s^2 2p^2$



(a) (b) (c)

In (a) & (b) the spins cancel out. Hence the configuration for C is (c)

Electronic Configuration of the Elements

- 1 H $1s^1$
- 2 He $1s^2$
- 3 Li $1s^2 2s^1$
- 4 Be $1s^2\ 2s^2$
- 5 B $1s^2\ 2s^2\ 2p^1$
- 6 C $1s^2\ 2s^2\ 2p^2$
- 7 N $1s^2\ 2s^2\ 2p^3$
- 8 O $1s^2\ 2s^2\ 2p^4$
- 9 F $1s^2\ 2s^2\ 2p^5$
- 10 Ne $1s^2\ 2s^2\ 2p^6$
- 11 Na $1s^2\ 2s^2\ 2p^6\ 3s^1$
- 12 Mg $1s^2\ 2s^2\ 2p^6\ 3s^2$
- 13 Al $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^1$
- 14 Si $1s^2\ 2s^2\ 2p^6\ 3s^2 3p^2$
- 15 P $1s^2\ 2s^2\ 2p^6\ 3s^2 3p^3$
- 16 S $1s^2\ 2s^2\ 2p^6\ 3s^2 3p^4$
- 17 Cl $1s^2\ 2s^2\ 2p^6\ 3s^2 3p^5$
- 18 Ar $1s^2\ 2s^2\ 2p^6\ 3s^2 3p^6$

The second period of the period table is made up of the elements Lithium (Li) to Neon (Ne)

Element	atomic number	electronic configuration
Lithium	3	$1s^2\ 2s^1$ $\boxed{\uparrow\downarrow}\ \boxed{\uparrow}$
Beryllium	4	$1s^2\ 2s^2$ $\boxed{\uparrow\downarrow}\ \boxed{\uparrow\downarrow}$
Boron	5	$1s^2\ 2s^2\ 2p^1$ $\boxed{\uparrow\downarrow}\ \boxed{\uparrow\downarrow}\ \boxed{\uparrow}\boxed{}\boxed{}$
Carbon	6	$1s^2\ 2s^2\ 2p^2$ $\boxed{\uparrow\downarrow}\ \boxed{\uparrow\downarrow}\ \boxed{\uparrow}\boxed{\uparrow}\boxed{}$
Nitrogen	7	$1s^2\ 2s^2\ 2p^3$ $\boxed{\uparrow\downarrow}\ \boxed{\uparrow\downarrow}\ \boxed{\uparrow}\boxed{\uparrow}\boxed{\uparrow}$
Oxygen	8	$1s^1\ 2s^2\ 2p^4$ $\boxed{\uparrow\downarrow}\ \boxed{\uparrow\downarrow}\ \boxed{\uparrow\downarrow}\boxed{\uparrow}\boxed{\uparrow}$

Work out the number of electrons that can simultaneous have (i) n= 3, l=2 (ii) n = 3

(i) When

n = 3

l = 2

m =	**-2,**	**-1**	**0**	**+1**	**+2**
s =	**±½**	**±½**	**±½**	**±½**	**±½**
	2 e	**2e**	**2e**	**2e**	**2e**

Total 10e

(i) When

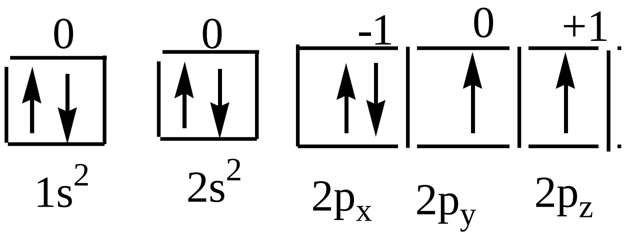
n = 3									
l =	**0**		**1**				**2**		
m =	**0**	**-1,**	**0,**	**+1**	**-2,**	**-1**	**0**	**+1**	**+2**
s =	**±½**	**±½**	**±½**	**±½**	**±½**	**±½**	**±½**	**±½**	**±½**
	2 e	**2e**	**2e**	**2e**	**2e**	**2e**	**2e**	**2e**	**2e**

Total 18e

Write down the four quantum numbers for each of 8 electrons in an Oxygen atom.

1. Write the electron configuration of the Oxygen atom.

$1s^2\ 2s^2\ 2p^4$

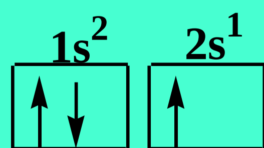


Electron	n	l	m	s
1	1	0	0	+½
2	1	0	0	-½
3	2	0	0	+½
4	2	0	0	-½
5	2	1	-1	+½
6	2	1	0	+½
7	2	1	+1	+½
8	2	1	-1	-½

Diamagnetism and Paramagnetism

PARAMAGNETISM: Ability to attract a magnet and characteristic of substances that contain net UNPAIRED electrons.

e.g. $_3$Li $1s^2\ 2s^1$



Li is therefore a paramagnetic compound

DIAMAGNETISM: Substances do not contain net unpaired electrons and REPELLED by magnet.

e.g. $_{20}$Ca [Ar]$4s^2$

Ca is therefore diamagnetic

Fisher Scientific

Periodic Chart of the Elements

1	2	3	4	5	6	7	8	9	10	11	12	•13	14	15	16	17	18	
IA IA	IIA IIA	IIIA IIIB	IVA IVB	VA VB	VIA VIB	VIIA VIIB	VIIIA VIIIB	VIIIA VIIIB	VIIIA VIIIB	IB IB	IIB IIB	◆13 ▪IIIB ★IIIA	14 IVB IVA	15 VB VA	16 VIB VIA	17 VIIB VIIA	18 0 VIIIA	
		3d	4d	5d	6d	7d	8d	9d	10d	11d	12d							
1 H 1.00794△																1 H 1.00794△	2 He 4.002602*	2
3 Li 6.941*	4 Be 9.01218											5 B 10.811△	6 C 12.011	7 N 14.0067	8 O 15.9994†	9 F 18.998403	10 Ne 20.179	2 8
11 Na 22.98977	12 Mg 24.305											13 Al 26.98154	14 Si 28.0855†	15 P 30.97376	16 S 32.066△	17 Cl 35.453	18 Ar 39.948	2 8 8
19 K 39.0983	20 Ca 40.078△	21 Sc 44.95591	22 Ti 47.88†	23 V 50.9415	24 Cr 51.9961△	25 Mn 54.9380	26 Fe 55.847†	27 Co 58.9332	28 Ni 58.69	29 Cu 63.546†	30 Zn 65.39*	31 Ga 69.723△	32 Ge 72.59†	33 As 74.9216	34 Se 78.96†	35 Br 79.904	36 Kr 83.80	2 8 18 8
37 Rb 85.4678†	38 Sr 87.62	39 Y 88.9059	40 Zr 91.224*	41 Nb 92.9064	42 Mo 95.94	43 Tc (98)	44 Ru 101.07*	45 Rh 102.9055	46 Pd 106.42	47 Ag 107.8682†	48 Cd 112.41	49 In 114.82	50 Sn 118.710△	51 Sb 121.75†	52 Te 127.60†	53 I 126.9045	54 Xe 131.29†	2 8 18 18 8
55 Cs 132.9054	56 Ba 137.33	57 **La 138.9055†	72 Hf 178.49†	73 Ta 180.9479	74 W 183.85†	75 Re 186.207	76 Os 190.2	77 Ir 192.22†	78 Pt 195.08†	79 Au 196.9665	80 Hg 200.59†	81 Tl 204.383	82 Pb 207.2	83 Bi 208.9804	84 Po (209)	85 At (210)	86 Rn (222)	2 8 18 32 18 8
87 Fr (223)	88 Ra 226.0254	89 ▼Ac 227.0278	104 Unq§ (261)	105 Unp§ (262)	106 Unh§ (263)													

• New IUPAC
▪ Former IUPAC
◆ New Chemical Abstract Service
★ Former Chemical Abstract Service

**Lanthanides

58 Ce 140.12	59 Pr 140.9077	60 Nd 144.24†	61 Pm (145)	62 Sm 150.36†	63 Eu 151.96	64 Gd 157.25†	65 Tb 158.9254	66 Dy 162.50†	67 Ho 164.9304	68 Er 167.26†	69 Tm 168.9342	70 Yb 173.04†	71 Lu 174.967	2 8 18 32 9 2

▼Actinides

90 Th 232.0381	91 Pa 231.0359	92 U 238.0289	93 Np 237.0482	94 Pu (244)	95 Am (243)	96 Cm (247)	97 Bk (247)	98 Cf (251)	99 Es (252)	100 Fm (257)	101 Md (258)	102 No (259)	103 Lr (260)	2 8 18 32 32 9 2

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§The International Union of Pure and Applied Chemistry (IUPAC) has not adopted official names or symbols for these elements.

*These weights are considered reliable to ±2 in the last place.

†These weights are considered reliable to ±3 in the last place.

△These weights are considered reliable in the last place, as follows: Calcium and Gallium ±4; Boron ±5; Chromium and Sulfur ±6; Hydrogen and Tin ±7.

All other weights are reliable to ±1 in the last place. All reliabilities are based on an uncertainty scale of ±1 to 9.

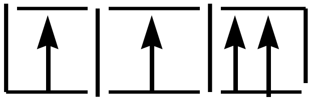
Atomic weights corrected to conform to the most recent values of the Commission on Atomic Weights. Column nomenclature conforms to IUPAC system and data in this chart have been checked by the National Bureau of Standards' Office of Standard Reference Data.

ELECTRONIC CONFIGURATION

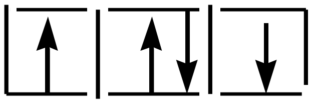
- Note:
- 1. The **s-block** elements
- 2. The **p- block** elements
- 3. The **d-block** elements.

Tutorial (A)

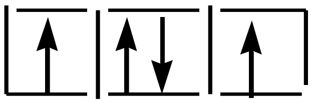
Examine the orbital diagrams which represents the ground-state electronic configuration of certain elements. Which of them violate the Pauli Exclusion principle? Hund's rule?



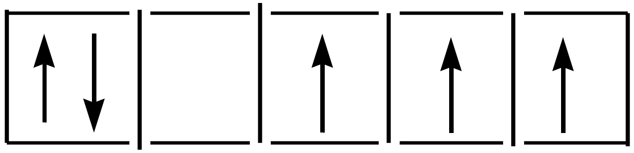
(a)



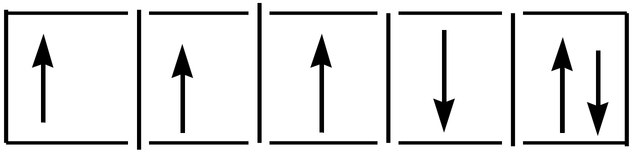
(b)



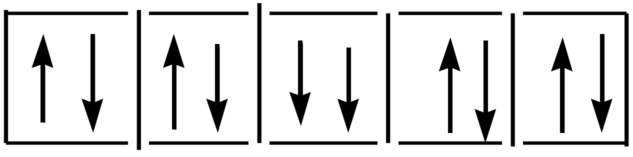
(c)



(d)



(e)



(f)

TUTORIAL (B):

What is the maximum number of electrons in an atom that can have the follow quantum numbers:
(a) $n = 2$, $m_s = -\frac{1}{2}$ (b) $n = 5$, $l = 3$; (c) $n = 4$, $l = 3$, $m_l = -3$;

TUTORIAL (C):
An ion has the electronic configuration:

$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^2$

(i) Write the electronic configuration for the neutral atom
(ii) How many unpaired electrons are in the neutral atom.

ANSWER:

(a) and (f) violate Pauli's Exclusion Principle

(b) :   (b), (d) and (e) violate Hund's rule

Read it and weep

A boy applied for a job as a public bathroom attendant. He was told he would be given the job after he filled out the form, but the boy replied that he could not write. Then interviewer informed him that he did not qualify.

On his way home, the boy saw some apples that were underpriced and bought them. He sold them for double the price.

As the years passed, he ended up becoming a millionaire who owned a chain of 20 fruit stores.

One day his bank manager asked him to sign some papers.
“Sorry” he said “I can’t write. My wife looks after that.”

You are kidding! said the bank manager. “What would you have become if you could write?”

The millionaire thought for a moment and said: “a public bathroom attendant.”

END

- THIS IS THE END OF THIS SESSION.
- I HOPE WE ARE ALL FOLLOWING.
- PLEASE FEEL FREE TO ASK ANY QUESTIONS.