Quantum numbers and Shapes of orbitals.

Quantum numbers

(1) Each orbital in an atom is specified by a set of three quantum numbers (n, l, and m) and each electron is designated by a set of four quantum numbers (n, l, m and s).

(2) Principle quantum number (n)

(I) It was proposed by Bohr's and denoted by 'n'.

(ii) It determines the average distance between electron and nucleus, means it is denoted the size of atom.

$$r = \frac{n^2}{Z} \times 0.529\ \mathring{A}$$

(iii) It determine the energy of the electron in an orbit where electron is present.

$$E = -\frac{Z^2}{n^2} \times 313.3\ Kcal\ per\ mole$$

(iv) The maximum number of an electron in an orbit represented by this quantum number as $2n^2$. No energy shell in atoms of known elements possess more than 32 electrons.

(v) It gives the information of orbit K, L, M, N------------.

(vi) The value of energy increases with the increasing value of n.

(vii) It represents the major energy shell or orbit to which the electron belongs.

(viii) Angular momentum can also be calculated using principle quantum number

$$mvr = \frac{nh}{2\pi}$$

(3) Azimuthal quantum number (l)

(I) Azimuthal quantum number is also known as angular quantum number. Proposed by Sommerfield and denoted by 'l'.

(ii) It determines the number of sub shells or sublevels to which the electron belongs.

(iii) It tells about the shape of subshells.

(iv) It also expresses the energies of subshells $s < p < d < f$ (increasing energy).

(v) The value of $l = (n-1)$ always where 'n' is the number of principle shell.

(vi)					
Value of l	=	0	1	2	3..........(n-1)
Name of subshell	=	s	p	d	f
Shape of subshell	=	Spherical	Dumbbell	Double dumbbell	Complex

(vii) It represent the orbital angular momentum. Which is equal to $\frac{h}{2\pi}\sqrt{l(l+1)}$

(viii) The maximum number of electrons in subshell $= 2(2l+1)$

$s-$ subshell $\rightarrow$ 2 electrons $d-$ subshell $\rightarrow$ 10 electrons

$p-$ subshell $\rightarrow$ 6 electrons $f-$ subshell $\rightarrow$ 14 electrons.

(ix) For a given value of 'n' the total value of 'l' is always equal to the value of 'n'.

(x) The energy of any electron is depend on the value of n & l because total energy = (n + l). The electron enters in that sub orbit whose (n + l) value or the value of energy is less.

(4) Magnetic quantum number (m)

(I) It was proposed by Zeeman and denoted by 'm'.

(ii) It gives the number of permitted orientation of subshells.

(iii) The value of m varies from –l to +l through zero.

(iv) It tells about the splitting of spectral lines in the magnetic field i.e. this quantum number proved the Zeeman effect.

(v) For a given value of 'n' the total value of 'm' is equal to n^2.

(vi) For a given value of 'l' the total value of 'm' is equal to $(2l+1)$.

(vii) Degenerate orbitals: Orbitals having the same energy are known as degenerate orbitals. E.g. for p subshell p_x p_y p_z

(viii) The number of degenerate orbitals of s subshell =0.

(5) Spin quantum numbers (s)

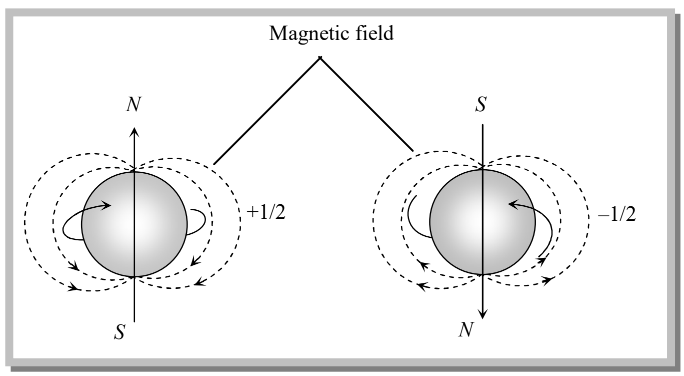
(I) It was proposed by Goldshmidt & Ulen Back and denoted by the symbol of ‘s’.

(ii) The value of $'s'$ is $+1/2$ and $-1/2$, which is signifies the spin or rotation or direction of electron on its axis during movement.

(iii) The spin may be clockwise or anticlockwise.

(iv) It represents the value of spin angular momentum is equal to $\frac{h}{2\pi}\sqrt{s(s+1)}$.

(v) Maximum spin of an atom $=1/2\times$ number of unpaired electron.



(vi) This quantum number is not the result of solution of Schrodinger equation as solved for H-atom.

Distribution of electrons among the quantum levels

n	l	m	s	Designation of orbitals	Electrons present	Total no. of electrons
1 (K shell)	0	0	+1/2, −1/2	1s	2	2
2 (L shell)	0 1	0 +1 0 −1	$+1/2, -1/2$ $+1/2, -1/2$ $+1/2, -1/2$ $+1/2, -1/2$	2s 2p	2 6	8

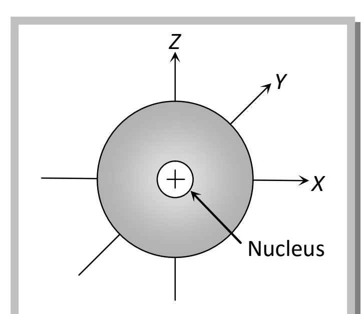
3 (M shell)	0	0	$+1/2, -1/2$	3s	2	
			$+1/2, -1/2$			
		+1	$+1/2, -1/2$		6	
	1	0	$+1/2, -1/2$	3p		
		−1				
			$+1/2, -1/2$			18
			$+1/2, -1/2$			
			$+1/2, -1/2$			
		+2	$+1/2, -1/2$		10	
		+1	$+1/2, -1/2$	3d		
	2	0			2	
		−1	$+1/2, -1/2$			
			$+1/2, -1/2$		6	
		−2	$+1/2, -1/2$			
	0	0	$+1/2, -1/2$	4s		
		+1				
	1	0		4p		
		−1	$+1/2, -1/2$		10	
			$+1/2, -1/2$			
			$+1/2, -1/2$			
			$+1/2, -1/2$			
			$+1/2, -1/2$			
		+2				
		+1	$+1/2, -1/2$		14	
	2	0	$+1/2, -1/2$	4d		32
			$+1/2, -1/2$			
		−1	$+1/2, -1/2$			
			$+1/2, -1/2$			
		−2	$+1/2, -1/2$			
4(N shell)			$+1/2, -1/2$			
			$+1/2, -1/2$			
		+3				
		+2				
		+1				
	3	+0		4f		

		−1				
		−2				
		−3				

Shape of orbitals

(1) Shape of ‘s’ orbital

(I) For ‘s’ orbital l=0 & m=0 so ‘s’ orbital have only one unidirectional orientation i.e. the probability of finding the electrons is same in all directions.



(ii) The size and energy of 's' orbital with increasing 'n' will be $1s < 2s < 3s < 4s$.

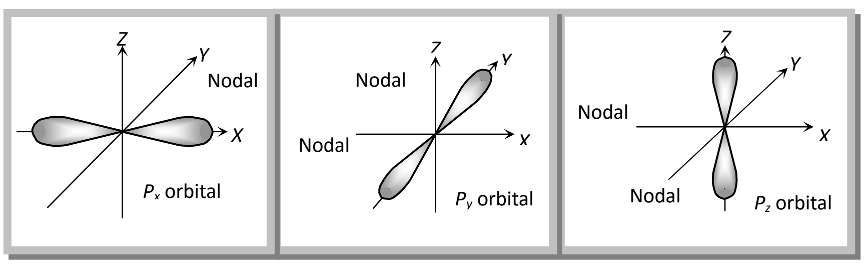
(iii) It does not possess any directional property. S orbital has spherical shape.

(2) Shape of 'p' orbitals

(I) For 'p' orbital l=1, & m=+1,0,–1 means there are three 'p' orbitals, which is symbolized as p_x, p_y, p_z.

(ii) Shape of 'p' orbital is dumb bell in which the two lobes on opposite side separated by the nodal plane.

(iii) p-orbital has directional properties.



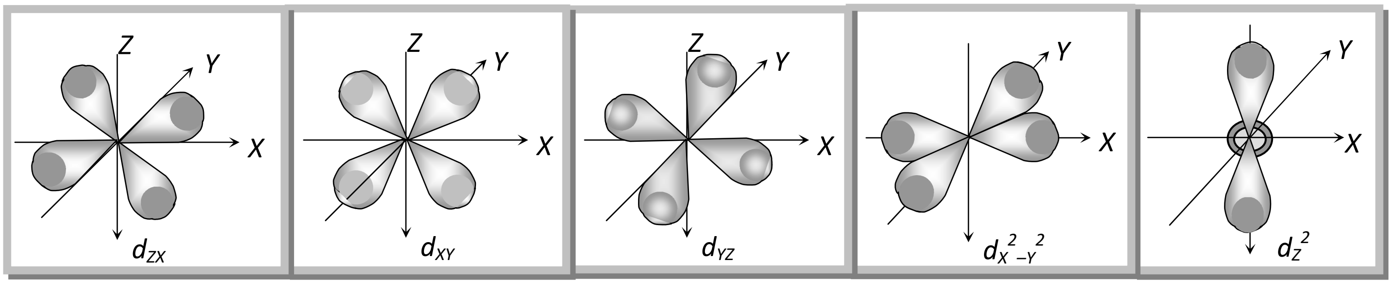
(3) Shape of'd' orbital

(I) For the 'd' orbital l =2 then the values of 'm' are –2,–1,0,+1,+2. It shows that the 'd' orbitals has five orbitals as $d_{xy}, d_{yz}, d_{zx}, d_{x^2-y^2}, d_{z^2}$.

(ii) Each 'd' orbital identical in shape, size and energy.

(iii) The shape of d orbital is double dumb bell.

(iv) It has directional properties.



(4) Shape of 'f' orbital

(I) For the 'f' orbital l=3 then the values of 'm' are –3, –2, –1,0,+1,+2,+3. It shows that the 'f' orbitals have seven orientation as $f_{x(x^2-y^2)}, f_{y(x^2-y^2)}, f_{z(x^2-y^2)}, f_{xyz}, f_{z^3}, f_{yz^3}$ and f_{xz^2}.

(ii) The 'f' orbital is complicated in shape.