QUANTUM NUMBERS

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An atom contains a large number of orbitals. These are distinguished from each other on the basis of their size, shape and orientation in space. These characteristics of an orbital are expressed in term of three numbers, called principal, azimuthal and magnetic quantum numbers. These numbers also follow form the solution of the Schrodiger wave equation. Further, to represent the spin (rotation) of the electron about its own axis, a fourth quantum number, called spin quantum number is introduced by Uhlenbeck and Goudsmit in 1925. ***Thus , Quantum numbers may be defined as a set of four numbers with the help of which we can get complete information about all the electron in an atom, i.e., location, energy, the type of orbital occupied, shape and orientation of that orbital, etc.***

These numbers are like the postal address of a man. To know about a particular person, Mr. X, we should know his country, his town, his lane and his house number. The four quantum numbers are briefly discussed below:

1. **Principal Quantum Number (n).** It is the most important quantum number since it tells the principal energy level or shell to which the electron belongs. It is denoted by the letter 'n' and can have any integral value except zero, i.e., n= 1,2,3,4 ... etc. The various principal energy shell are also designated by the letter, K, L, M, N, O, P ... etc. starting from the nucleus. This number helps to explain the main lines of the spectrum on the basis of the electronic jumps between these shells. The principal quantum number gives us the following information:
   (i) it gives the average distance of the electron from the nucleus. In other words, it largely determines the size of the electron cloud.
   (ii)it completely determines the energy of the electron in hydrogen atom and hydrogen like particles (which contain only one electron). For example, the energy of the electron in the nth shell of the hydrogen atom is given by $E_n = -2\pi^2me^4/n^2h^2$ where m is the mass, e is the charge of the electron and h is Planck's constant. However, in case of multi-electron atoms, it determines only the approximate energy of any electron.
   For the first principal shell (K), n = 1 which means that this energy shell is of lowest energy and lies closest to the nucleus. For the second principal shell (M), n = 2 and for the third principal shell (M), n =3 and so on. The energies of the various principal shells follow the sequence:
   K < L< M < N < O < P .... Or 1 < 2< 3< 4< 5 .....
   (iii) the maximum number of electrons present in any principal shell is given by $2n^2$ where n is the number of the principal shell.

2. **Azimuthal or angular momentum quantum number (l**). It is found that the spectra of the elements contain not only the main lines but there are many fine lines also present. To explain the presence of these fine lines, it was suggested that the electrons present in any main shell of a multi-electron atom do not have the same energy. This is because they move along different angular momentum. Thus, within the same principal shell, there are present a number of sub-shell or sub-levels of energy. As a result, the number of electronic jumps increases and so is the number of lines. Thus, this number helps to explain the fine lines of the spectrum.
   The azimuthal quantum number gives the following information:
   (i) The number of sub-shells present in the main shell.
   (ii)The angular momentum of the electron present in any sub-shell.
   (iii) The relative energies of the various sub-shell.
   (iv) The shape of the various sub-shells present within the same principal shell.

   This quantum number is denoted by the letter 'l'. For a given value of n, it can have any intergral value ranging from 0 to n-l. For example, for the 1st shell(K), n = 1, l can have only one value ,i.e., l= 0 ,for the 2nd shell (L), n=2, l can have two value, i.e., l= 0 and 1 ,for the 3rd shell (M), n=3, l can have three value, i.e., l = 0,1 and 2 , for the 4th shell (N), n=4, l can have four value, i.e., l = 0, 1 , 2, and 3.

   Each value of 'l' represents a different sub-shell. Depending upon the value of l, i.e., l= 0, 1, 2, and 3, the different sub-shell are designated as s, p, d, f respectively. These notations are the initial letter of the words, sharp, principal, diffused and fundamental. To sum up :

Value of 'l'	0	1	2	3	4	5
Designation	s	p	d	f	g	h

of sub-shell							

(i) n = 1, l = 0 1s
(ii) n =2, l =0,1 2s 2p
(iii) n = 3, l = 0,1,2 3s 3p 3d
(iv) n = 4, l = 0, 1, 2, 3, 4s 4p 4d 4f

Thus, in general, the number of sub-shells present in any principal shell is equal to the number of the principal shell or the principal quantum number.

Further, the energies of the different sub-shells present within the same principal shell are found to be in order s<p<d<f i.e., an electron in the s-subshell has lower energy than that in the p-sub-shell of the same principal shell. Angular momentum of the electron in an orbital = $\sqrt{l(l+1)}$ h/2π

3. **Magnetic Quantum Number (m or m_l).** This quantum number is required to explain the fact that when the source producing the line spectrum is placed in a magnetic field, each spectral line splits up into a number of lines (Zeeman effect). This may be explained as follow:
An electron due to its orbital motion around the nucleus generates an electric field. This electric field in turn produces a magnetic field which can interact with the external magnetic field. Thus, under the influence of the external magnetic field, the electrons of a subshell can orient themselves in certain preferred region of space around the nucleus called orbitals. The magnetic quantum number determines the number of preferred orientation of the electrons present in a subshell. Since each orientation corresponds to an orbital, therefore the magnetic quantum number determines the number of orbitals present in any subshell. The magnetic quantum number is denoted by the letter 'm' and for a given value of l, it can have all the values ranging from –l to +l including zero, i.e., -l, -(l-1), -(l-2).... 0, 1....(l-2), (l-1), l . Thus, for every value of l,m has 2l+1 values. For example, (i) For l = 0 (s-sub-shell) , m can have only one value, i.e., m= 0. This means that s-sub-shell has only one orientation in space. In other words, s-sub-shell has only one orbital called s-orbital. (ii) For l = 1 (p-sub-shell), m can have three values, i.e., m = -1, 0, +1. This means that p-sub-shell has three orientations in space. In other words, a p-sub-shell has three orbital. Since these three orbital are oriented along x-axis, y-axis and z-axis, therefore, they are commonly referred to as p_x p_y and p_z. (iii) For l =2 (d-sub-shell), m can have five values, i.e., m = -2, -1, 0, +1 and +2. This implies that there are five different orientations of d-sub-shell in space. In other words, d-sub-shell has five d-orbitals. (iv) Similarly, when l=3 (f-sub-shell), m can have seven values, i.e., m = -3, -2, -1, 0, +1 +2, and +3. This implies that there are seven different orientations of the f-sub-shell. In other words, f-sub-shell has seven f-orbitals.

To sum up:

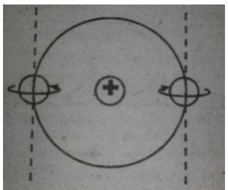
Sub-shell	s	p	d	f	g
No. of orbitals present	1	3	5	7	9

Values of m by latest conventions

Orbital	Value of m	Orbital	Value of m
p_z	m = 0	d_{z^2}	m = 0
p_x	m= +1	d_{xz}	m = +1
p_y	m = -1	d_{yz}	m = -1
		$d_{x^2-y^2}$	m = +2
		d_{xy}	m = -2

It may be pointed out that all the three p-orbitals of a particular principal shell have the same energy in the absence of a magnetic field. Similarly, all the five d-orbitals of a particular shell have same energy. These orbital of the same sub-shell having equal energy are called degenerate orbitals. However, in presence of an external magnetic field, this degeneracy is broken or split and the orbitals of the same sub-shell acquire slightly different energies. This causes the splitting of a given spectral line into many.

4. Spin quantum number (s). This number was introduced to account for the fact that the electron in an atom not only moves around the nucleus but also spin about its own axis (like the earth which not only revolves around the sun but also spin around its own axis). This number gives the information about the direction of spinning of the electron present in any orbital. It is represented by 's'. since the electron in an orbital can spin either in the clockwise direction or in the anti-clockwise direction, hence for a given value of m , s can have only two values, i.e., +1/2 and -1/2 or these are very often represent by two arrows pointing in the opposite direction, i.e., ↑ and ↓ .



Spinning of electrons.

This quantum number helps to explain the magnectic properties of the substances. A spinning electron behaves like a micromagnet with a definite magnetic moment. If an orbital contains two electrons, the two magnetic moments oppose and cancel each other.

Thus ,it may be concluded that :

No. of sub-shells in nth shell = n

No. of orbital in a sub-shell = 2l+1

Maximum no. of electrons in a subshell =2(2l+1)

No.of orbitals in nth shell =n^2

Maximum no. of electrons in nth shell = $2n^2$

ASSIGNMENT

1. For a d- electron, the orbital angular momentum is :
   (a) $\sqrt{6}\hbar$ (b) $\sqrt{2}\hbar$ (c) $\hbar$ (d) $2\hbar$
2. The total number of orbitals in a shell having principal quantum number n is
   (a) 2n (b) n^2 (c) $2n^2$ (d) n+1
3. The maximum number of electrons in an orbit with l=2, n=3 is
   (a) 2 (b) 6 (c) 12 (d) 10
4. Not possible is
   (a) n=3 , l=0, m=0 (b) n=3, l=1, m=-1
   (c) n=2, l=0, m=-1 (d) n=2, l=1, m=0.
5. The orbitals for n=3, l=2 , m=+2
   (a) 1 (b) 2 (c) 3 (d) 4
6. The total number of orbitals for principal quantum number n=4, having l=3 is
   (a) 3 (b) 5 (c) 7 (d) 9
7. The number of 2p electrons having spin quantum number s = -1/2 are
   (a) 6 (b) 0 (c) 2 (d) 3
8. If n=3, l=0, m=0, then atomic number is
   (a) 12, 13 (b) 13, 14 (c) 10 , 11 (d) 11, 12

Answers : 1. (a) 2. (b) 3. (d) 4. (c) 5. (a) 6. (c) 7. (d) 8. (d)