

# Structure of atom

## Visible rays

It is the part of the spectrum that is detected by the human eye. It runs from about  $4 \times 10^{14}$  Hz to about  $7 \times 10^{14}$  Hz or a wavelength range of about 700- 400 nm. Visible light emitted or reflected from objects around us provides us information about the world. Our eyes are sensitive to this range of wavelengths. Different animals are sensitive to different range of wavelengths. For example, snakes can detect infrared waves, and the visible range of many insects extends well into the ultraviolet.

## Definition

### Electromagnetic spectrum

The different types of electromagnetic radiations differ only in the wavelengths and hence frequencies. Their wavelengths increase in the following order.

Cosmic rays <  $\gamma$  rays < X-rays < Ultra-violet rays < Visible < Infrared < Micro waves < Radio waves

## Definition

### Spectrum

The band of colours (VIBGYOR) seen on passing the white light through a prism is called the spectrum.

## Diagram

### White light spectrum

White light is nothing but colourless day light. This contains all the wavelengths of the visible spectrum at equal intensity. In simple terms, electromagnetic radiation of all the frequencies in the visible range of the spectrum, appearing white to the eye is called white light.

Visible light or white light is the part of the electromagnetic spectrum which can be detected by the human eye.

## Developments leading to the Bohr's model of atom

It is observed that all elements give characteristic line spectra which could not be explained on the basis of Rutherford's model. For this, it is essential to understand the nature of light for which electromagnetic theory and Planck's quantum theory is necessary. Hence a new model called Bohr's model of atom was put forward.

## Bohr's Model of Atom

Back in 20th century, scientists made several attempts to explain the structure of atom. Although unsuccessful, Rutherford's model of atom played a key role in discovery of a much successful model which was given by Neil Bohr in 1913. The Rutherford model had a major drawback; it could not explain why electrons do not fall into the nucleus by taking a spiral path. It was in line with the electromagnetic theory which says "if a charged particle undergoes accelerated motion, then it must radiate energy (lose) continuously". Bohr proposed the Quantum Theory of Atom. He retained some key postulates of Rutherford and added some points using Quantum Physics. Hence, his model is also known as Rutherford-Bohr model.

### Postulates of Bohr's atomic model

Following are the principal postulates of Bohr's Atomic Model:

1. According to Quantum Physics, when an electron is revolving in a particular orbit or particular energy level around the nucleus, the electron does not radiate energy even though it has accelerated motion around the nucleus. Hence Neil Bohr proposed that, the electrons could revolve around the nucleus in only 'certain orbits' (energy levels) having nucleus at its center. Each orbit has a different radius and certain energy associated with it.
2. Bohr proposed that the angular momentum of an electron is quantized. Thus, the motion of an electron is restricted to those orbits where its angular momentum is an integral multiple of  $\frac{h}{2\pi}$ , where  $h$  is Planck's constant. Hence, we have the relationship  $mvr = n\frac{h}{2\pi}$ , where  $m$  is mass of electron,  $v$  is velocity of electron of said orbit,  $r$  is radius of that orbit,  $n$  is a simple integer.
3. The stationary states or allowed energy levels are only those where  $n = 1, 2, 3$ , This is called Bohr quantum condition. It essentially tells you that energy levels of an atom are quantized, meaning electron can only reside in certain energy levels of an atom.
4. The energy of an electron changes only when it moves from one orbit to another. An electronic transition from an inner orbit to outer orbit involves absorption of energy. Similarly, when an electron jumps from an outer orbit to inner orbit it releases energy, which is equal to the difference between the two energy levels.
5. The energy thus released in the form of a radiation of a certain frequency appears in the form of a line in the atomic spectrum. If the energy of an electron in the outer orbit ( $n_2$ ) is  $E_2$  and energy of electron in the inner orbit ( $n_1$ ) is  $E_1$  then  $E_2 - E_1 = \Delta E = h\nu$ .
6. The value of  $n$  could be small integers 1, 2, 3 corresponding to the first, second, third shell and so on. Quantum states are shells for the electron and  $n$  is termed as principal quantum number.

## Features of quantum mechanical model

The energy of electrons in an atom is quantised (i.e., electrons can only have certain specific values of energy).

The existence of quantised electronic energy states is a direct result of the wave-like property of electrons.

The exact position and the exact velocity of an electron in an atom cannot be determined simultaneously (Heisenberg uncertainty principle).

An atomic orbital is represented by the wave function  $\psi$ , for an electron in an atom, and is associated with a certain amount of energy.

There can be many orbitals in an atom, but an orbital cannot contain more than two electrons.

The orbital wave function  $\psi$  gives all the information about an electron.

$|\psi|^2$  is known as probability density, and from its value at different points within an atom, the probable region for finding an electron around the nucleus can be predicted.

## Definition

### Quantum numbers

A number that occurs in the theoretical expression for the value of some quantized property of a subatomic particle, atom, or molecule and can only have certain integral or half-integral values is called as quantum number, e.g., Principle quantum numbers, Azimuthal quantum numbers, spin quantum numbers.

### Principle quantum number

The principal quantum number  $n$ , designates the principal electron shell. Because  $n$  describes the most probable distance of the electrons from the nucleus, the larger the number  $n$  is, the farther the electron is from the nucleus, the larger the size of the orbital, and the larger the atom is.  $n$  can be any positive integer starting at 1, as  $n=1$  designates the first principal shell (the innermost shell). The first principal shell is also called the ground state, or lowest energy state. This explains why  $n$  can not be 0 or any negative integer, because there exists no atoms with zero or a negative amount of energy levels/principal shells.

### Azimuthal quantum numbers

The orbital angular momentum quantum number  $l$  determines the shape of an orbital, and therefore the angular distribution. The number of angular nodes is equal to the value of the angular momentum quantum number  $l$ . Each value of  $l$  indicates a specific s, p, d, f sub-shell (each unique in shape.) The value of  $l$  is dependent on the principal quantum number  $n$ . Unlike  $n$ , the value of  $l$  can be zero. It can also be a positive integer, but it cannot be larger than one less than the principal quantum number ( $n-1$ ):  $l=0,1,2,3,4,(n-1)$

### Subshell

One or more orbitals in the electron shell of an atom with the same energy level. Subshells have different shapes and are distinguished by their magnetic quantum number. e.g 1s, 2s, 2p, 3d.

## Orbitals

An atomic orbital is a mathematical function that describes the wave-like behavior of either one electron or a pair of electrons in an atom. This function can be used to calculate the probability of finding any electron of an atom in any specific region around the atom's nucleus. For example: 1s represent 1st orbit with s orbital.

## Magnetic quantum number

The magnetic quantum number  $m_l$  determines the number of orbitals and their orientation within a sub-shell. Consequently, its value depends on the orbital angular momentum quantum number  $l$ . Given a certain  $l$ ,  $m_l$  is an interval ranging from  $l$  to  $+l$ , so it can be zero, a negative integer, or a positive integer.

$$m_l = l, (l+1), (l+2), \dots, 2, 1, 0, 1, 2, (l-1), (l-2), +l$$

## Spin quantum number

Spin quantum number designates the direction of the electron spin and may have a spin of  $+1/2$ , represented by  $\uparrow$ , or  $1/2$ , represented by  $\downarrow$ . Unlike  $n$ ,  $l$ , and  $m_l$  the electron spin quantum number  $m_s$  does not depend on another quantum number. This means that when  $m_s$  is positive the electron has an upward spin, which can be referred to as "spin up." When it is negative, the electron has a downward spin, so it is "spin down." The significance of the electron spin quantum number is its determination of an atom's ability to generate a magnetic field or not.

## Solve problems on quantum numbers

What designations are given to the following orbitals having.

A.  $n=2, l=1$

Solution : when  $n=2$  and  $l=1$  the orbital is 2p.

B.  $n=1$  and  $l=0$ .

solution : when  $n=1$  and  $l=0$  the orbital is 1s.

## Process of filling of electrons

When an atom or ion receives electrons into its orbitals, the orbitals and shells fill up in a particular manner. The rules of filling of electrons are: Aufbau's rule, Hund's rule, Pauli's exclusive principle, orbital order

## Aufbau Principle

Orbitals with the lowest principal quantum number ( $n$ ) have the lowest energy and will fill up first. Within a shell, there may be several orbitals with the same principal quantum number. In that case, more specific rules must be applied. For example, the three p orbitals of a given shell all occur at the same energy level. So, how are they filled up? ans: all the three p orbitals have same energy so while filling the p orbitals we can fill any one of the  $P_x$ ,  $P_y$  or  $P_z$  first. it is a convention that we chose to fill  $P_x$  first, then  $P_y$  and then  $P_z$  for our simplicity. Hence you can opt for filling these three orbitals from right to left also.

### Hund's rule of maximum multiplicity

According to Hund's rule, orbitals of the same energy are each filled with one electron before filling any with a second. Also, these first electrons have the same spin. This rule is sometimes called the "bus seating rule". As people load onto a bus, each person takes his own seat, sitting alone. Only after all the seats have been filled will people start doubling up.

### Electronic configuration of elements

Electronic configuration of any element is given by general electronic configuration

$1s^2 2s^2 2p^x 3s^y \dots$ .....For example : Sodium has atomic number 11. The electronic configuration of sodium is  $1s^2 2s^2 2p^6 3s^1$ .

### Full filled and half filled

There are two reasons of stability-

1. Symmetry- half filled and fully filled sub-shells lead to symmetry and symmetry always increases stability in the nature.
2. Exchange energy- In half filled and fully filled sub-shells there are maximum no. of exchanges which releases energy hence increasing stability. Exchange of e<sup>-</sup>s also can be understood as delocalization of e<sup>-</sup>s which is similar like resonance and resonance always increases stability.

### Exchange energy

Exchange energy is the energy released when two or more electrons with the same spin exchange their positions in the degenerate orbitals of a sub-shell. Let's assume an atom in which there are 5 unpaired electrons(i.e one unpaired electron in each one ) in its n d-orbital.