Inductively Coupled Plasma Atomic Emission Spectrometry (ICP-AES) for Pollution Monitoring

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Lecture – 05
Course introduction and atomic structure – V

Greetings to you! In the last 2 classes, we have had some sort of introduction to the environmental pollution monitoring and then atom Inductively Coupled Plasma Atomic Emission Spectroscopy. And then as part of it go, we have decided to look at the structure of the atom and what we have covered in the previous class is the discovery of the fundamental particles of the atomic structure and the nuclear arrangement.

The nuclear arrangement basically consists of protons and neutrons held together by colonic forces and van der Waals forces etcetera. And we have also discussed the stability of the nucleus depending upon the structure of the protons and neutrons. We also discussed about the isotopes. Now subsequently we have this, we have moved to the outer arrangement of the electrons. And we have said that Bohr's theory, Daltons theory and Rutherford's theory etcetera all these things refer to the arrangement of electrons around the nucleus.

And the size of this electronic arrangement, the space around which the electrons orbit around the nucleus is approximately 10000 times larger than the size of the nucleus. So, we have also said that the movement of the electrons from one orbit to another orbit is the reason for the transition of the elements, transition of the electrons, 2 different orbitals and these transitions are governed by quantum mechanical rules and the quantum mechanical rules, according to Bohr's theory can be interpreted and each line spectra for hydrogen atom has been ascribed to 5 different series. And the, we have discussed that it is the exact quantity of energy corresponding to the difference in each orbit that corresponds to the movement of the electron.

So, if all the electrons fall to the principal quantum number shell that is n is equal to 1, we have what is known as Lyman series.

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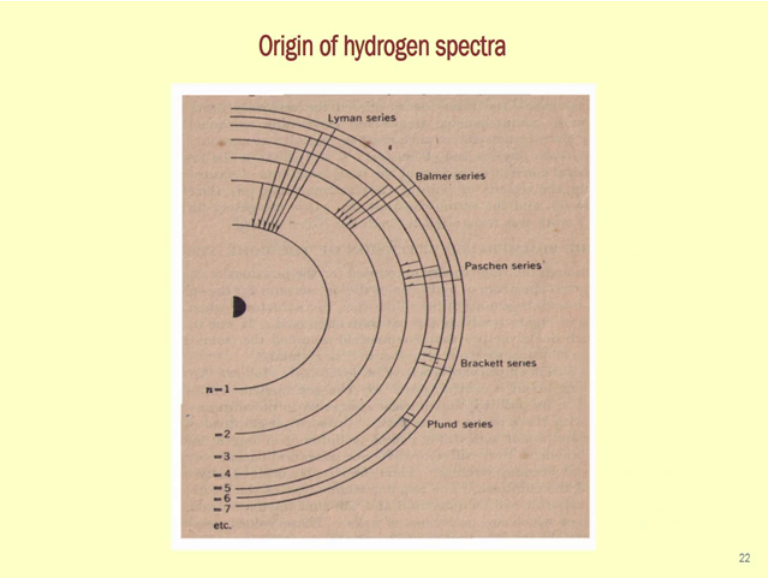

And so, we this here it is the n is equal to 1, here it is 2, 3, 4 like that; these are the different orbitals and this falls in UV and vacuum ultraviolet region followed by if the electrons fall on to the second shell, then we have what is known as Balmer series and Balmer series is occurs in the visible range, similarly Paschen series where the electrons fall to the third shell around the nucleus; that is Paschen series that is in near IR and IR and then followed by Bracket series and Front series.

So, n is equal to 4, 5, 6, 7 etcetera. We have different kinds of transitions occurring around the electron which can be interpreted like this. we also said that the electrons process around themselves also and for each electron we need to describe a position which is denoted by 4 different quantum numbers that is n, l, m and s.

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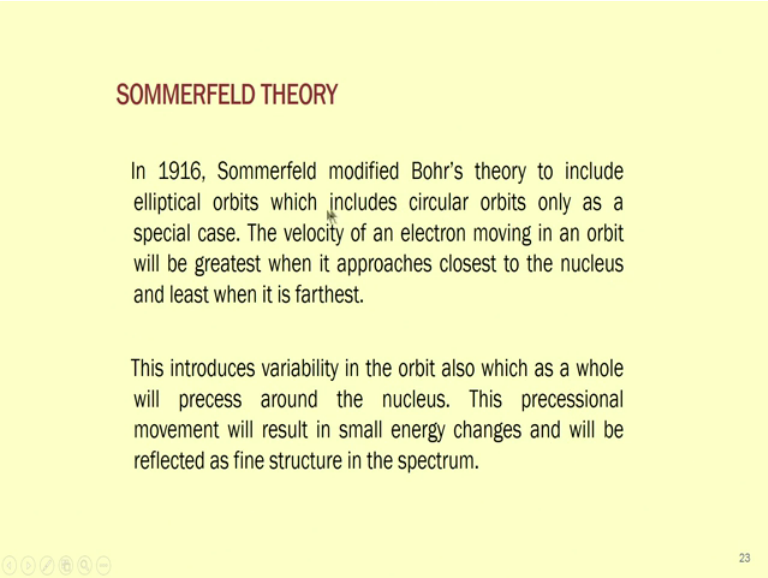

So, the Sommerfeld Theory, modified Bohr's theory to include some elliptical orbits. So, he just said unlike Bohr's theory, all the electrons are revolving around the nucleus in circular orbits, but he modified it to elliptical orbits.

And the elliptical orbit is a special case of a circular orbit is a special case of elliptical orbit because any elliptical orbit is defined by 2 parameters a and b; and when a is equal to b then, we have circular orbit. So, you can look up your basic mathematics structure studies to find out the nature of elliptical orbits and circular orbit; suffice it to say that circular orbit is only a special case and that happens only in the case of hydrogen. And the velocity of the electron moving in an orbit will be greatest as it approaches closest to the nucleus and least when it is farther.

This is another concept of the Sommerfeld Theory. What he says is, as the electron moves nearer the nucleus, the speed of the electron increases. As it moves away, it is it decreases. This is somewhat similar situation regarding the planets. The planet arrangement of around the sun also follow elliptical orbits and whenever the any planet comes very near the sun this speed of the planet increases and it tends to move farther and farther away faster towards farther distances.

As it comes, as it moves farther away, the speed decreases. So, essentially similar arrangement he has proposed, Sommerfeld. And this introduces variability the in the orbit also which as a whole will process around a nucleus. So, this precessional

movement will result in small energy changes and it will be reflected in the fine structure of the spectrum also. So, the Sommerfeld theory's contribution to the spectroscopy is that, there will be small energy changes which are reflected in the spectroscopic fingerprint of all the elements.

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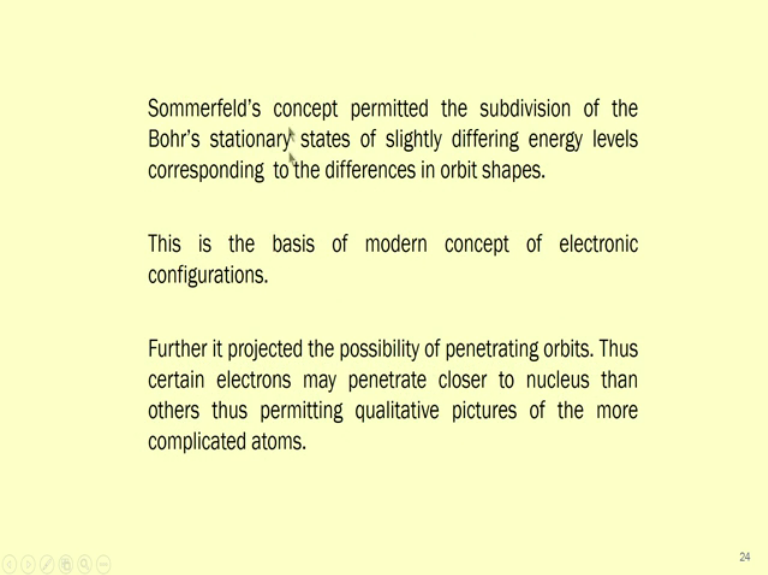

So, this permitted the subdivision of the Bohr's stationary states of slightly different energy levels corresponding to the differences in orbit shapes. So right now, as of now this is the basis of modern concept of electronic configurations; that means, whenever we want to build the electrons around the nucleus, that is if you remember your high school chemistry periodic table is there, all the elements are arranged according to their atomic weight and atomic number.

And if you want to know, how the electrons are hydrogen has 1, lithium has 2, helium is 2 lithium is 3 like that beryllium, boron, carbon, nitrogen, oxygen, sulfur, all those things have 1 electron each extra added to each element. And the basis of modern concept of electronic, how the electrons are arranged around the nucleus is based on Sommerfeld's Theory.

So, it projected the possibility of penetrating objects also; that means the orbit is basically a space around the nucleus. So, 2 orbits can interact, they can intersect each other depending upon the their shapes; that means, the different electrons can occupy this common orbitals at different times. So, what we are saying essentially is over a period of

time there will be time waited energy density around their nucleus in a specific area in a around the nucleus in a specific volume.

So, that is what whenever 2 shapes are intermixing each other, the possibility of 2 electrons or more electrons around that area space is much more. So, that is when we call the orbits are penetrating each other. So, we have some sort of a qualitative picture of the more complicated atoms also.

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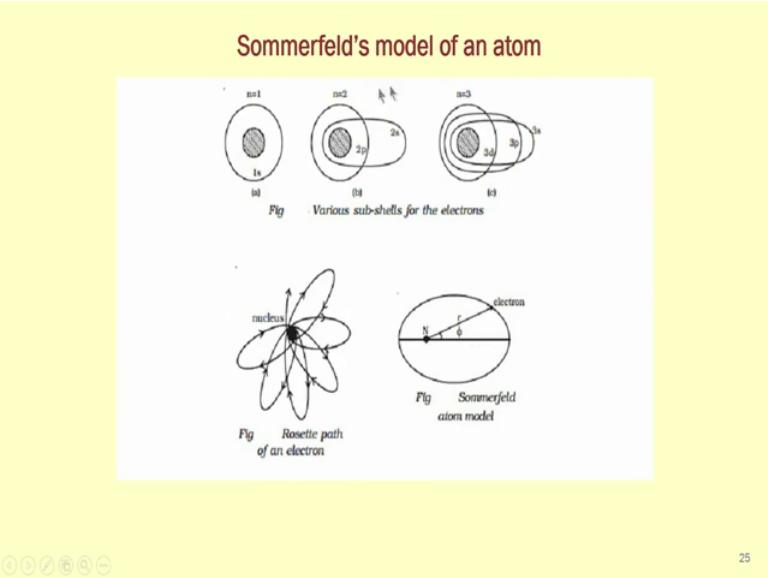

So, this is the Summerfeld's model of an atom. And you can see that the when n is equal to 1, the orbit is exactly circular, spherical; actually the orbit is circular, but the space around the nucleus is spherical; that means, you will be able to find the electron in this space all over the space, but not above, beyond this space, where I have written a circular circle defined a circle.

Now, when the n is equal to 2, we need to have 2 orbits and you can see that the circular part remains the same and there is a 2p and 2s also. So, this 2s orbital is a, 1s is circular, as ours spherical and 2s is elliptical. And you keep on compressing elliptical nearer towards this side, you will end up with a circular space. So, the actual orbit is 2s and 2p also there is another possibility. Now, in 3s, we have when n is equal to 3, we have 3s, 3p and 3d orbitals.

Similarly, if it is n is equal to 4 we have, 4s, 4p, 4d and 4 s; like that the you can see that there is certain amount of overlapping; for example, if you look at this area the overlapping of n is equal to 1 and n is equal to 2, there is certain area in which the spaces overlap; that means, the probability of finding an electron to finding both electrons in this area exists. Similarly there is more overlapping and as the electron, as the we keep on adding electrons along the periodic table, the things become very complicated.

And then it is the electron can be moving in any of these areas in any direction also and this is known as Rosette path of an electron. Now this is basically a Sommerfeld model, that is this is the nucleus, this is the electron. Electron is revolving around the nucleus and it is in the elliptical orbital. The orbit is an elliptical orbit.

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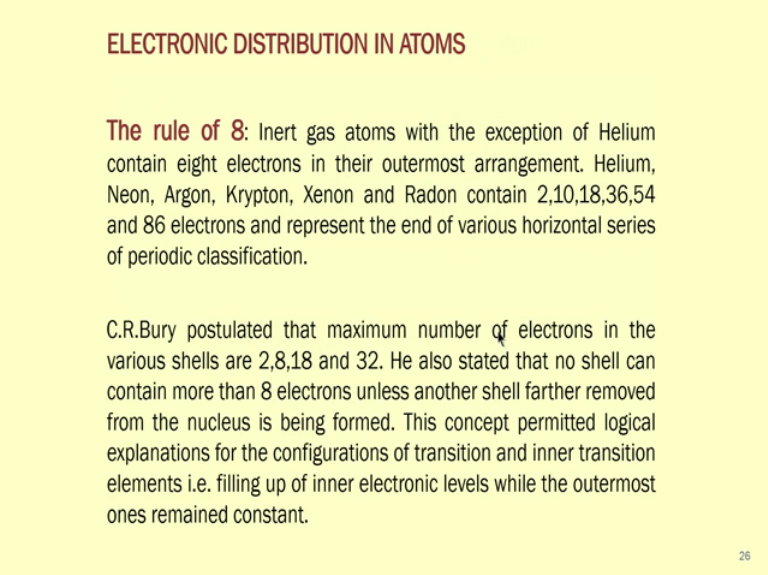

So, the distribution of electrons in the atoms is somewhat slightly more involved. I think all of this you would have studied at your p u c level. So, what we are going to do now, is basically to define the rules not go into more theoretical aspects so that we have a clear understanding of the atomic structure. So, first thing we have to know is about the rule of 8, that is the inert gas atoms with the exception of Helium contain 8 electrons in their outermost arrangement minimum, maximum 8.

For example helium has got only 2. All the electrons which are having less than 8, the rule does not apply of course, and Neon, Argon, Krypton, Xenon, etcetera all they Radon, these elements if you which you find in the periodic table to the extreme right,

they all have 2 electrons and then 10 electrons, 18, 36 and 54 and 86 electrons also are there in radon. So, they represent the end of a reserve various horizontal series of periodic classification.

So, this rule of 8 whenever there are 8 electrons in the outermost orbit, it represents a complete structure of the electrons and the element is a neutral element, for example, this Helium, Neon, Argon, Krypton, Xenon and Radon, they are all neutral elements. They do not carry any charge and they are very stable in inner, they are also known as inert gas elements. So, they are they do not undergo many chemical reactions and all this because the electronic arrangement is in such a way that there is no exchange of electrons or energy between the inert elements and other elements.

So, you know C R Bury, this is the name of another scientist, he postulated that maximum number of electrons in the various shells are 2, 8, 18 and 32. He also stated at that time Xenon and Radon etcetera they were not discovered. That is why he said 32 is the last this thing. He also stated that no shell can contain more than 8 electrons unless another shell further removed from the nucleus is being formed.

So, this concept permitted logical explanation for the configuration of transition and inner transition elements. We will study about the arrangement of the electrons in the periodic table further, what a what actually this means, but I am, I suspect that most of you already know about these things. So, we are not going to elaborate, but we will touch upon this later.

So, the transition and inner transition elements are part of the periodic table where filling up of inner electronic levels takes place while the outermost orbit contain the same number of electrons.

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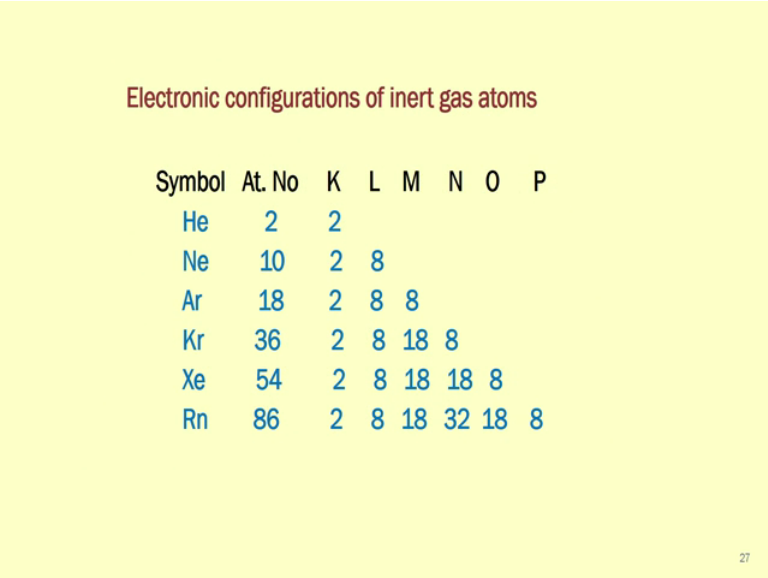

So, how do we look at the electronic arrangement of these inert elements? Here I have written the symbol Helium, Neon, Argon, Krypton, Xenon and Radon, this is the atomic number. So, number of protons or electrons are there. So, if there are 2 electrons, there it will have only 1 orbit and that is k shell, 1 shell then it can contain maximum 2 electrons.

Then comes the rule of 8. So, you move the move to Neon, it has got 10 electrons; the first will contain 2 next will contain 8. And go to Argon, that is the third inert element that we know and it contains 18 electrons the electronic arrangement will be 2, 8 and 8 there is 10 plus 8 is 18. Similarly go for Krypton that is 2, 8, 18 and 8. So, that you can always see that the last orbit, last shell will have only 8 electrons whatever is the number of electrons in the inner shells; same thing is true with the Xenon and same thing is true with Radon.

So, the rule of 8 is followed very rigorously in the periodic table while filling the electrons.

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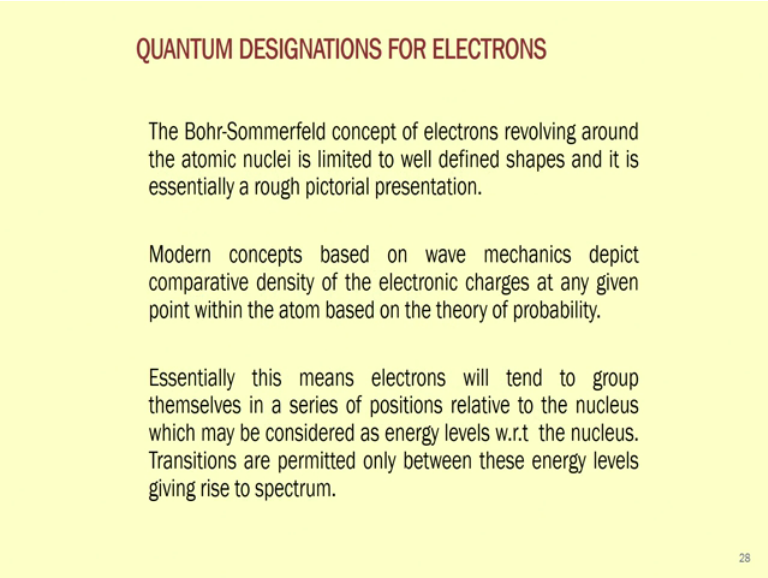

So, the Bohr-Sommerfeld concept of electrons revolving around the atomic nuclei is definitely you know related to well defined shapes and it is essentially a rough practical pictorial presentation. Obviously, the we cannot define a space around their nucleus in which the electron keeps on moving, in what exactly, it cannot be traced as a as if you are tracing, if a ball is moving around you tie a string to the ball and then move it around, your eye can pinpoint wherever it is there.

But with electrons it does not happen. So, it is what it describes is a sort of shape and it is essentially a rough pictorial presentation. Even if you play with a string with a ball attached and you rotate it very fast, you will also see only a blur defining a particular shape. Look at the fan turning around you above your head and you can see you will not be able to see the shape of the fan blade, but it will show you some sort of a blurred picture of the total space in which the fan blades are moving.

So, essentially same thing happens here. Only thing is electrons are much smaller and the shapes are different. So, modern concepts are basically based on the wave mechanics that depict the density, the relative density of the electronic charge in any given space around the nucleus. So, at any given point within the atom, the electron density is based on the theory of probability rather than actual happening.

So, this means that electrons will tend to group themselves in a series of positions relative to the nucleus. So, they may be considered as energy level because if the electron

is concentrated in one particular area, that area will be having more negative charge; if it is less a density, it will have relatively less negative charge. So, basically it is sort of energy level in which we described that the electron is placed at such and such energy level around the nucleus; the third electron is in the s orbital, p orbital, d orbital something like that. And then the transitions are permitted only between these energy levels from one electron density to another electron density area, this gives rise to the spectrum because there will be number of energy levels and where the electron density is more.

So, from one energy level density electron will be moving to higher energy levels. When you excite atom and or they fall to the lower different, lower different energy by emitting the radiation emitting the energy 2 different movements, different lower level energy. So, these energy levels, any transition of electron gives rise to the spectrum.

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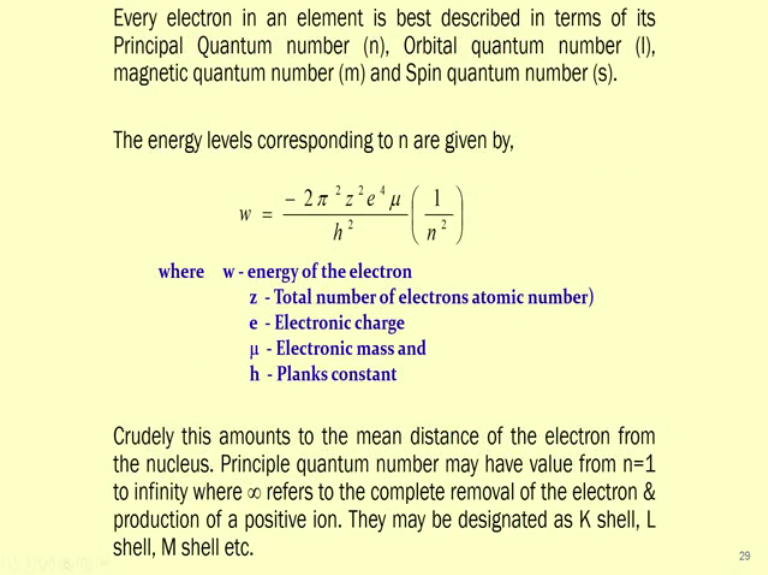

There. So, every electron in an element is described in terms of it is principal quantum number n and then orbital quantum number l and then magnetic quantum number m and spin quantum number s. It is better for you if you remember that every electron is a distinct electron in a given element.

So, the all the 4 quantum numbers, that is n, l, m and s are never same for any 2 electrons in a given element. So, that is how if n, m, n may be same, l may be same, magnetic quantum number m maybe same. If all the 3 are same, the 2 electrons that will

distinguish them only would be through the spin a like one is will be rotating around the positive axis, another is rotated will be rotating around the negative axis.

So, each electron around the nucleus is defined by 4 quantum numbers which are, which do not repeat for another electron in the same element. So, it is as if it has got a postal address wherein it is very distinct. So, the energy levels corresponding to the principal quantum number n is given by this equation, that is, w is the energy of equation minus 2 pi square z square e to the power of 4 and then you know the electronic mass multiplier divided by Planks constant multiplied by 1 over n square. That is if n is equal to 1, we have w would be exactly equal to 2 minus 2 pi square z square e to the power of 4 and then mass divided by Planks constant.

So, in this equation, it is better for us to remember that w is the energy of the electron and the z is the Total number of electrons or atomic number e is the Electronic charge, we know what is the number and mu is the Electronic mass and h is Planks constant. So, what this equation mean actually? Crudely, this energy w what we represent, it crudely amounts to the mean distance of the electron where if the probability of finding it is maximum and that distance is measured from the nucleus. So, that is the main distance at which an electron may be found.

And the principal quantum number in that equation is denoted by n know. So, the value of value of n can vary from 1 to infinity. So, n may be 1, n maybe 2, n is 3 like that. So, n square becomes less and less and when you divide it, when you divide 1 by n square, the distance becomes more and more. So, as the electron as a quantum principal quantum number n increases, the electron will be located farther and farther away from the nucleus.

So, you keep on removing the electron farther and farther away, at some point it will go out of the orbit of the electron. At that time we call it, it is ionized and electron is no more available around the nucleus and the nucleus is having excess positive charge there because the negative charge has been removed, but the new proton or neutron will not go away only the electron as gone away. So, the net charge will be positive. So, ion is it is called ion. So, principal quantum number varies, these are and they may be designated as k shell, l shell, m shell, etcetera ok.

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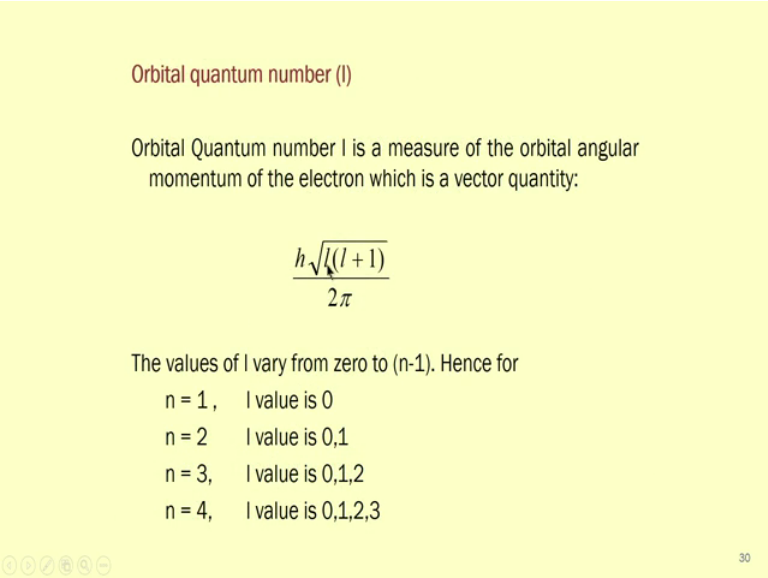

So as we have seen, k shell will have 2 electrons, l shell will have 10 electrons, like that there will be the different arrangement of electrons. Now we move on to the second identity of an electron that is denoted by Orbital Quantum number l. Now what is this Orbital Quantum number? I want you to understand that the shell that is n is equal to 1, n is equal to 2, etcetera, they represent circular area around the nucleus and that circular area keeps on increasing l is equal to, k is equal to, n is equal to 1; n is equal to 2 would be bigger, n is equal to 3 would be bigger circle. Like that the principal quantum number and it keeps on increasing.

Now, this orbital quantum number refers to the movement of the electron in that shell. So, because it is moving around the nucleus, the electron will be having orbital angular momentum. So, that is defined by this vector quantity h, that is Planks constant multiplied by square root of l into l plus 1 divided by 2 pi. So, the value of l varies from 0 to n minus 1. So, if n is equal to 1, n minus 1 would be 0. So, the value of l is 0; if n is equal to 2, the value of l would be 0 and 1.

Because n is equal to 2 means, n is equal to 1 also is there and second one also is there. For n is equal to 1, it is already 0; n is equal to 2, it will be n minus 1, would be 1. So, n is equal to 2 will have 2 orbitals corresponding to l is equal to 0 that is 1 orbital and another orbital corresponding to l is equal to 1. Similarly, if n is equal to 3, l will have 2 n plus 1, it will have 0, 1 and 2.

Similarly, n is equal to 4 would be having 0, 1, 2, 3, it will have 4 sub shells.

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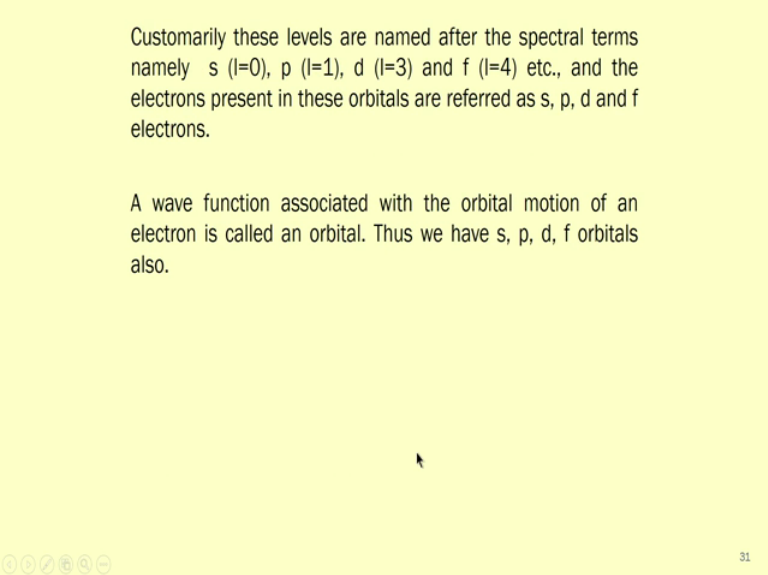

And customarily, these levels are named after these spectral terms s, p, d and f. So, l is equal to 0, these referred as a s orbital; l is equal to 1 is referred as p orbital and l is equal to 3 is referred as d orbital and f would be 4. So, the electrons present in these orbitals are referred as s, p, d, f electrons only.

Now, you should remember that this s orbital is circular. This p orbital where l is equal to 1 is like a dumbbell and d orbital also would be dumbbell, but with at different axis same is true with f orbitals also, that is different dumbbell shapes oriented in space around the nucleus. So, if you remember the dumbbell space, it will be like this 1 space above, 1 space below, in between the dumbbells there is a very thin line that is connecting the 2 spaces.

So, when you draw a dumbbell shape, it can be ascribed a mathematical equation just like a graph. So, the wave function is associated with the orbital motion of the electrons, that wave function is called as orbital. Thus we have s, p, d, f orbitals also. So, we define s is equal to 1, s orbital s electrons and it is also described by a mathematical equation which is given by s, p, d, f etcetera orbitals.

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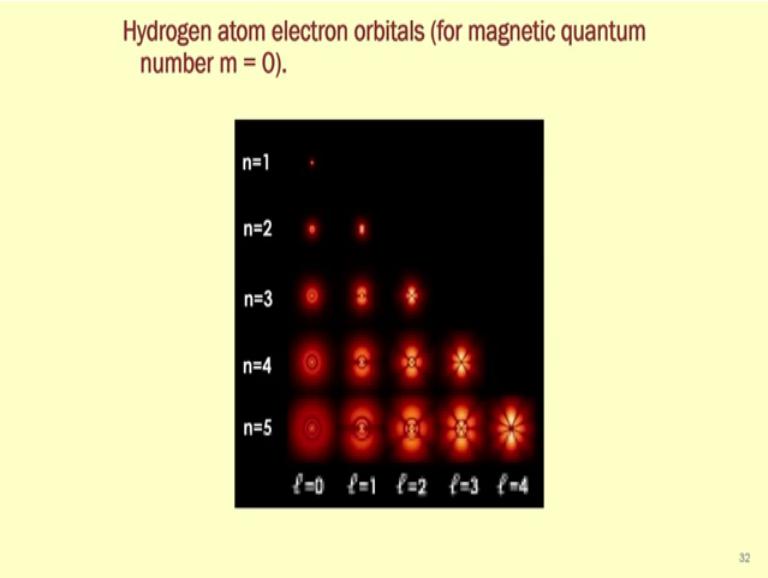

Now, this is how the electron n is equal to 1, n is equal to 2, n is equal to 3 are shown here. And this is for hydrogen atom, the electronic orbitals for magnetic quantum number m is equal to 0. So, when n is 1, you can see that there is a small red dot here. It is a circular this is the arrangement of electron. So, the electron would be around here. Then at the center of this dot, there is nucleus. So, when the n is equal to 2, we have l is equal to 0 and l is equal to 1 here. 0 is circular, l is equal to 1 would be sort of dumbbell shape. You can see more clearly, the same thing when n is equal to 3, we have a bigger one representing the size of the atom and then this is circular again; this is like a dumbbell shape and n is equal to l is equal to 2 would have is also like a dumbbell shape, but oriented differently in space.

So, n is equal to 4 same thing is true slightly clearer pictures, but more complicated because you have to remember that this is representing a space around the nucleus where the probability of finding the electron is more in these areas rather than in between somewhere here. In between the dumbbell shape the chances of finding the electrons as is very less. Same thing is true at n is equal to 5, n is equal to So, we have n is equal to 5, means l should be equal to 4. You can see that the shape is more diffused l is equal to 1, we have 2 dumbbell shape and then n is equal to 2, l is equal to 2 we have 4 dumbbells. Like that, the number of dumbbells will keep on increasing in the space around the nucleus.

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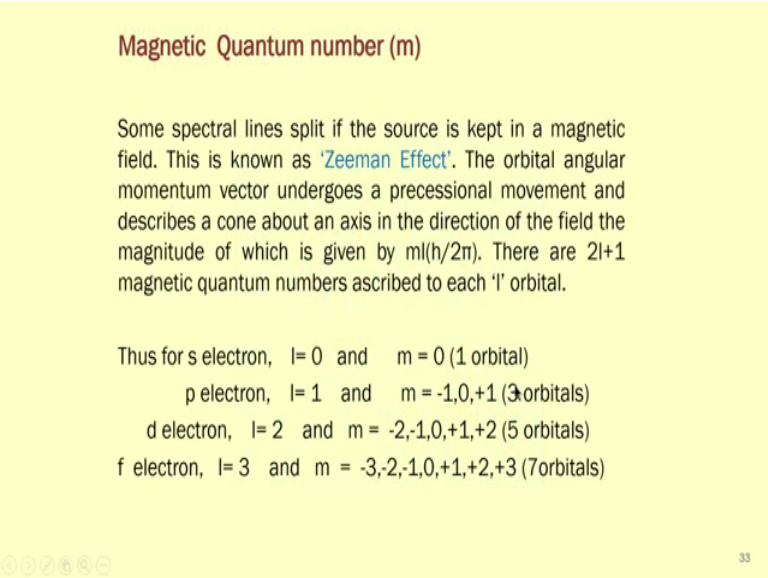

So will define the magnetic quantum number and spin quantum number in our next session.