Infrared Spectroscopy for Pollution Monitoring
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Lecture-07
Atomic Structure - IV

Greetings to you we were discussing about the quantum designations of the electrons, yesterday I was telling you that the every electron can be assigned an address in an electric, in an element whatever be the number of electrons. So the idea is no 2 electrons are similar have the same address, it is like IP address in computer. So, these addresses are defined as quantum numbers in atomic structure they are n, l, m and s.

N is the principle quantum number and l is the orbital angular momentum, m is the magnetic quantum number and s is the spin quantum number, we have already discussed all these things yesterday in the previous class.

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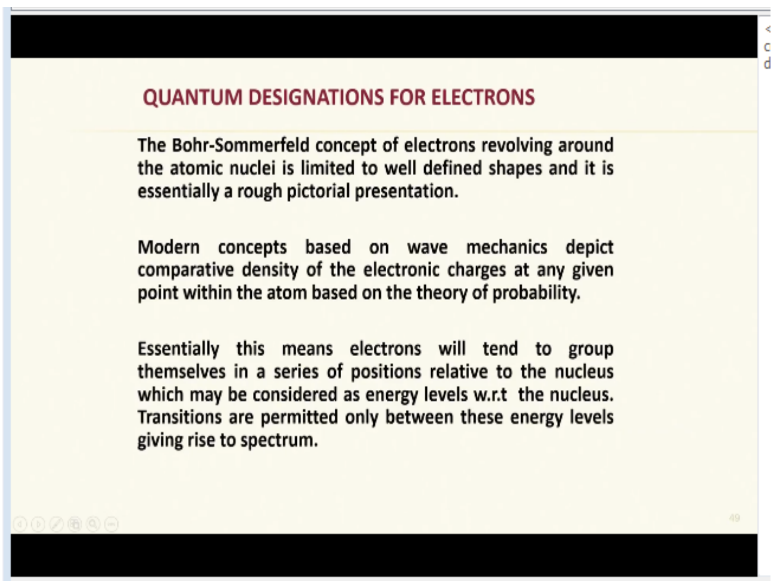

So, I have described about the principle quantum number this slide I had shown you followed by the orbital quantum number l.

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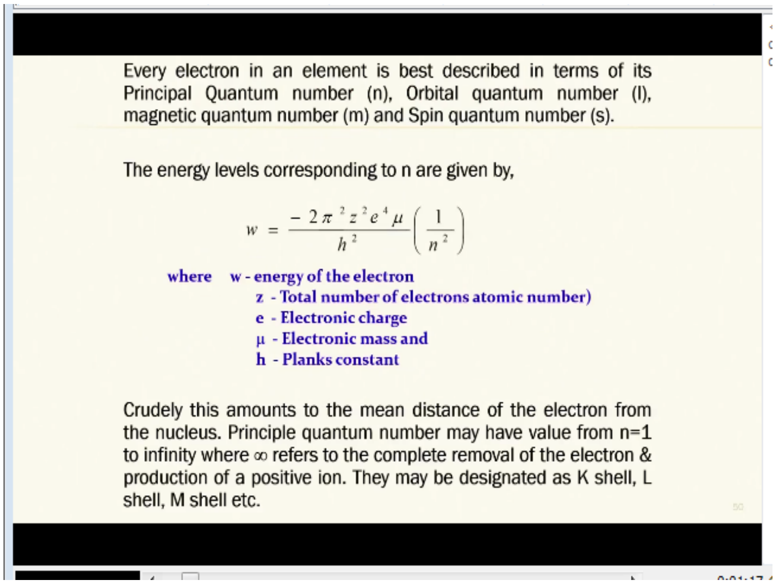

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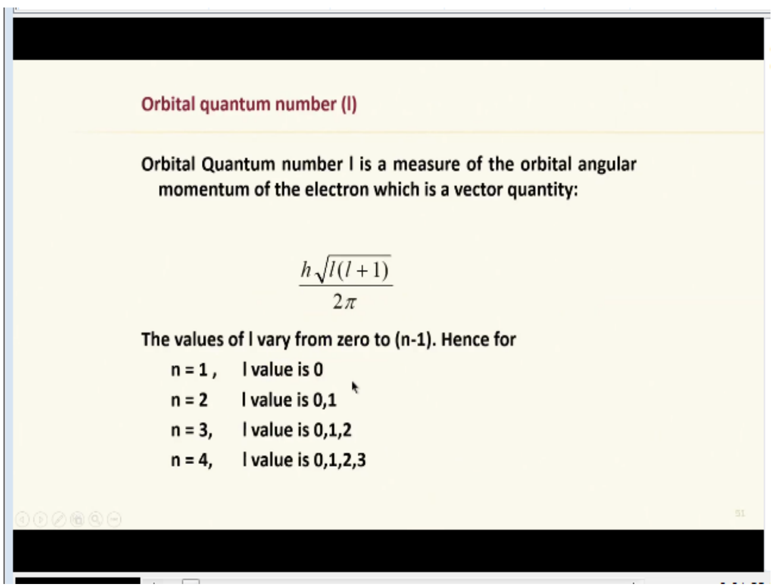

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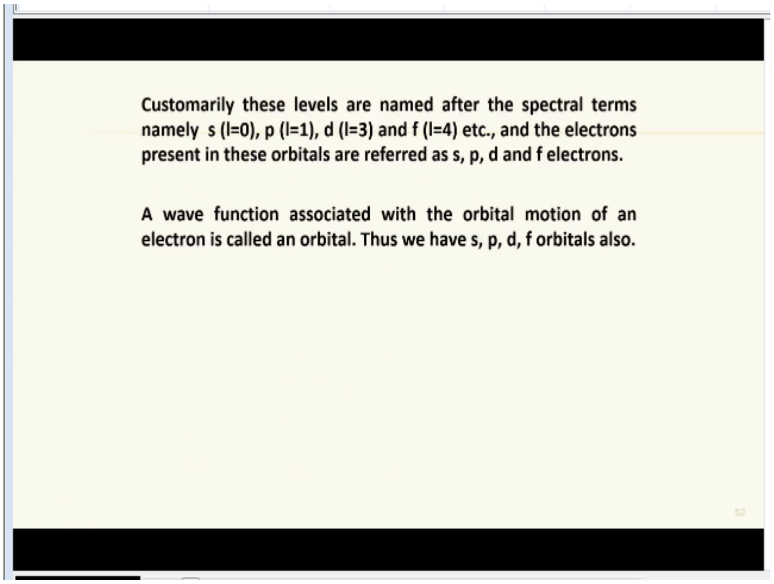

And then I had shown you the that the electrons are and orbitals are named as a p, d and f.

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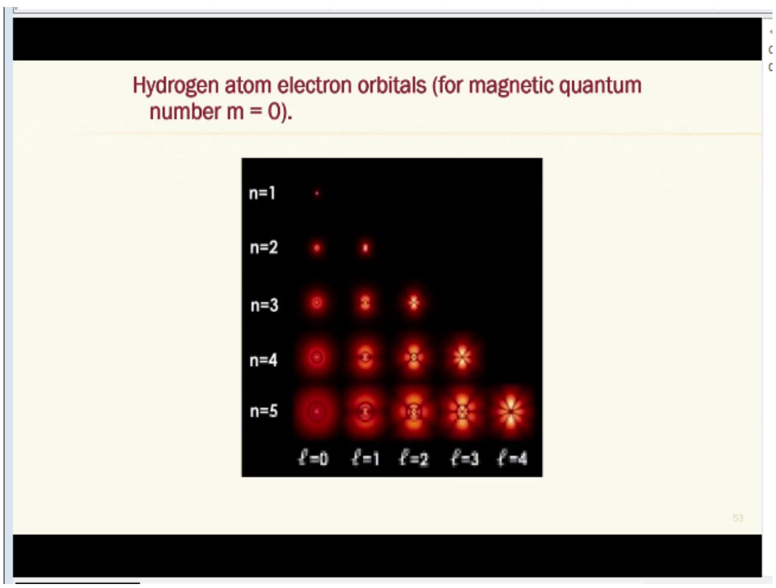

And then I had shown you this slide that corresponds to the different orbits or orbitals the electron orbitals in the hydrogen atom. And even though there is only one electron but the electron can occupy any of these orbitals. So at any time of the day or at any time the electron can be occupying m=0 sorry no n does not equal to 0. But n=1, n=2, n=3, n=4, n=5. And corresponding orbital angular momentum would be corresponding to l=0 to n-1 that is for the n is equal to 5 in the orbital angular momentum would be 4.

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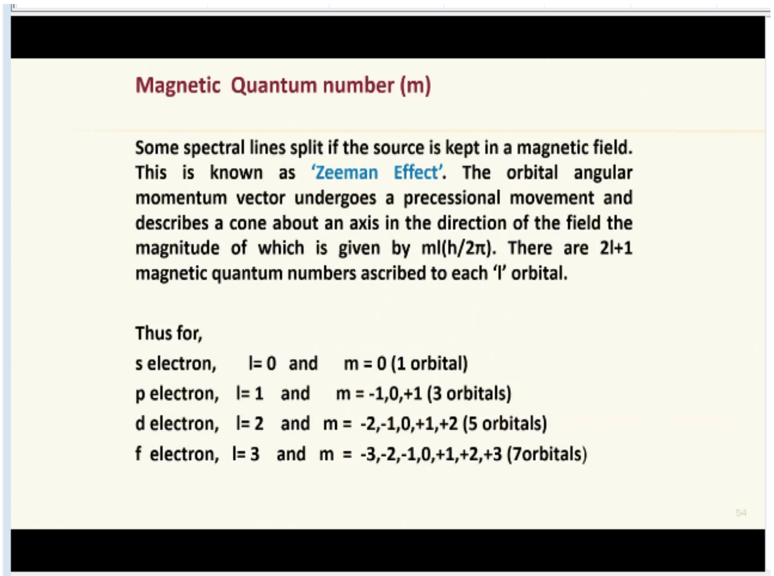

So, then I had also discussed a little bit about the magnetic quantum number and this magnetic quantum number makes lot of sense. If we consider that an electron is like a magnet, so if the magnetic effect can change the behavior of an electron. It should be reflect in the spectrum of hydrogen atom and that effect is known as Zeeman Effect. Yesterday we have discussed about this Zeeman Effect.

And then I had told you that under the magnetic field the electron orbital angular momentum vector itself undergoes a precessional movement that describes a cone about an axis in the direction of the field in which the magnitude of the momentum is given by ml*h/2 Pi all in all there are 2l+1 magnetic quantum numbers ascribed to each l orbital okay. Then I had discussed that l=0, m should be 0, and for p electrons there are 3 orbitals and for d electron there would be 5 orbitals.

And for f electron there would be 7 orbitals corresponding to magnetic different magnetic movements okay.

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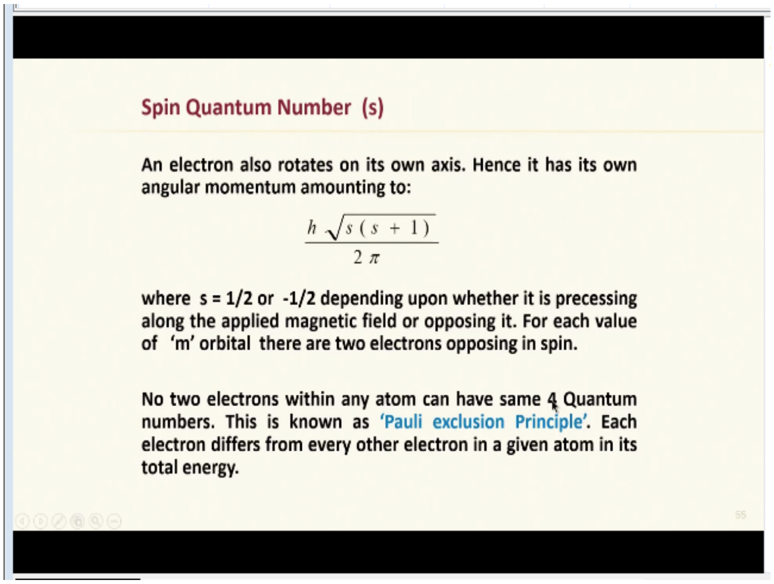

Now I want to discuss with you about the spin quantum number, so this spin is nothing to it is not unusual in our experience coming back to our solar system and the moments of the planets we assume that we know that the planets go round and round the sun in elliptical orbits and circular orbits etc. But also the precise round themselves, so exactly similar analogy is a existing in the atomic structure of the element that means each electron while it is going round and round the nucleus in its own prescribed through a path.

It will also be revolving around itself and that is known as spin quantum number. So the electron because it rotates on its own axis it has its own angular momentum also apart from the angular momentum that is the important by the moment of the by the magnetic field okay. So, that is quantified by this relation that is h*square root of s*s+1/2 Pi. So, where this s is spin quantum number the values of spin quantum numbers vary from =1/2 or -1/2.

This is by convention okay there are there is no hard and fast rule why it is +1/2 or why it is -1/2 or what is the significance or something like that. But in general it can be why there positive direction or it can be negative direction, another way of looking at it is either it can electron can spin in clock wise direction or anti-clockwise direction. If it is clock wise direction you call it positive, anti-clockwise you can call it negative depending upon the convention or your convenience.

But the excepted not is their spin quantum number is the approximate is actually 1/2. So, it can be +1/2 or -1/2 their nothing sacrosanct about 1/2 also. So, depending upon whether it is precessing along the applied magnetic field or opposing it. So, for each value of m orbital there are 2 electrons of opposing each other in the spin, so now you can appreciate that electrons within any atom can have same 4 quantum numbers.

Because the electrons are less total number of electrons in an element can be maximum 108 that is the number of elements and we can assign different quantum numbers. So, we make sure that every electron has a different IP address. So, this principle is known as Pauli exclusion principle that is each electron differs from every other electron in a given atom in its total energy. And the least it can differ from each other is by spin +1/2 or -1/2 okay.

So, the final composition of an electron or an element is that an element is composed of nucleus. And which is composed of protons and neutrons which is heavier and present at the center, center of gravity or whatever you call it of an element or of an atom. And an atom is having large empty space around it. And that empty space is populated by the number of electrons equal to the number of protons present in the element.

And the nucleus can also have different number of protons and different number of protons and varying number of neutrons. So, the number of there would be odd and even number of atomic weights for the same element called as an isotopes and coming back to the electron is electrons all the electrons can be assigned a fixed address in an element which can be fitted in any of the s, p, d, f and f orbitals.

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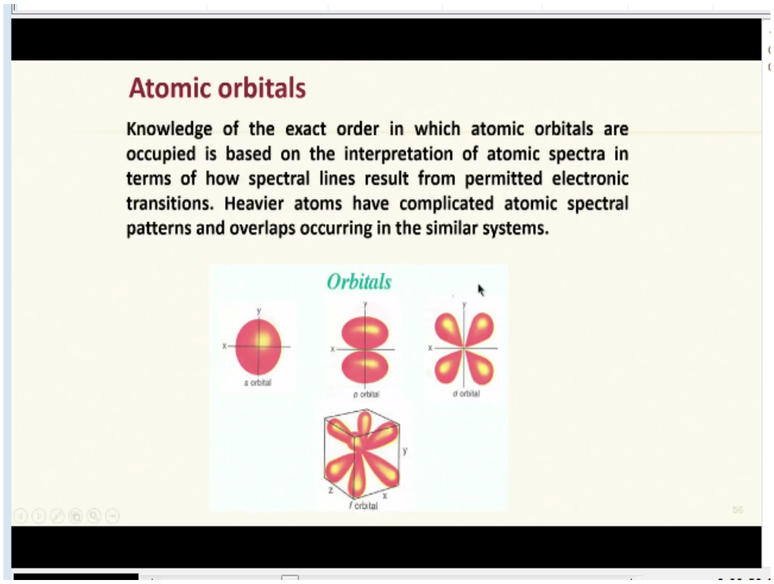

And every electron is different from each other, so that is where we are standing right now. And now I want to talk to you about the atomic orbitals, so as I was telling you the electrons must occupied different atomic orbitals. And we have seen that the electrons occupy s, p, d, f electrons but the knowledge of the exact order in which atomic orbitals are occupied is based on the interpretation of the atomic spectra in terms of how spectral lines result from the permitted electronic transitions.

This sentence makes lot of takes lot of significance there are 2 look at the slide now. Now the idea is there are 2 important concepts here, one is spectral lines result. And their result from permitted electronic transitions that means there are certain transitions that are not permitted or forbidden. So, heavier atoms have complicated atomic spectral patterns and it defeat is difficult to predict assign each and every spectral line corresponding to a particular transition of the electron in the spectrum okay.

And also the shape of each orbital also undergo the little bit of change because of the overlaps occurring in the similar systems. So, here I am showing you the different orbitals and I think most of since most of you are familiar. But for the sake of gravity I can say that s orbital is spherical in shape and it is in 3d volume 3d size. So, it is like a it covers the circular space around the nucleus with uniform radius or diameter whatever you call it.

So, first orbital 1s would be circular 2s should be circular slightly bigger circular bigger and 3s and 4s etc. would be of having similar shapes. Now coming to p orbitals, p orbitals have the shape of this duple**.** And then the population of electrons in the duples is higher. But not in the along the axis, so in the p orbital we have 3 p orbitals. One is located along x and y axis that is if you imagine if you imagine a plane something like this.

There would be one duple here another duple here. So, this is assumes that this is x-axis and this is y-axis. So, you call it xy, pxy, so another one is it can be like this one this it can be like this one behind you and one towards me, that is py, px, py and pz, pz is in the vertical space. One is the 2r along the horizontal space covered by x and y-axis and one would be in the vertical space. One above and one below the other 2 are 1 behind the other.

So, there are 3 p orbitals, and then we had d orbitals there should be theoretically 5d orbitals and there all distributed in different shapes along x, y and z orbitals. And the shapes are slightly complicated to imagine as such. But the general shape can be shown here like this okay. We will not going to detail because there are pair d x square, y square xy like that. There are 5 different d orbitals.

I could I have them but the f orbitals are also having 7 duple shape 4 at the top and 3 at the bottom. And again there will be more orbitals f orbitals and the combined effect of all these orbitals present around the nucleus in the space around it makes the whole system a bit complicated to imagine needs separate entity. So, all you would see if you if I project the atomic structure of an element he just a blurred area in which electrons are moving around it but it is the combined effect of all these orbitals which are having exact shapes.

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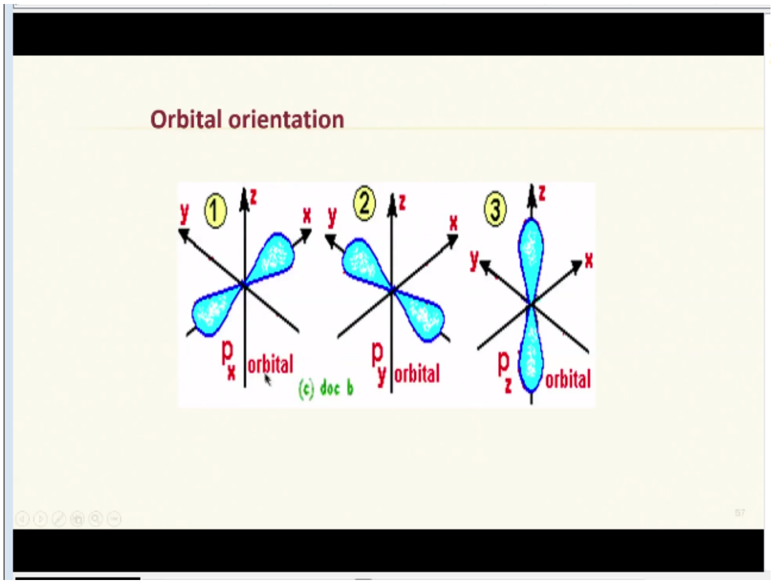

So, for example this px orbital p orbitals for example these are located along x-axis and then this is y-axis this is I have already told you know.

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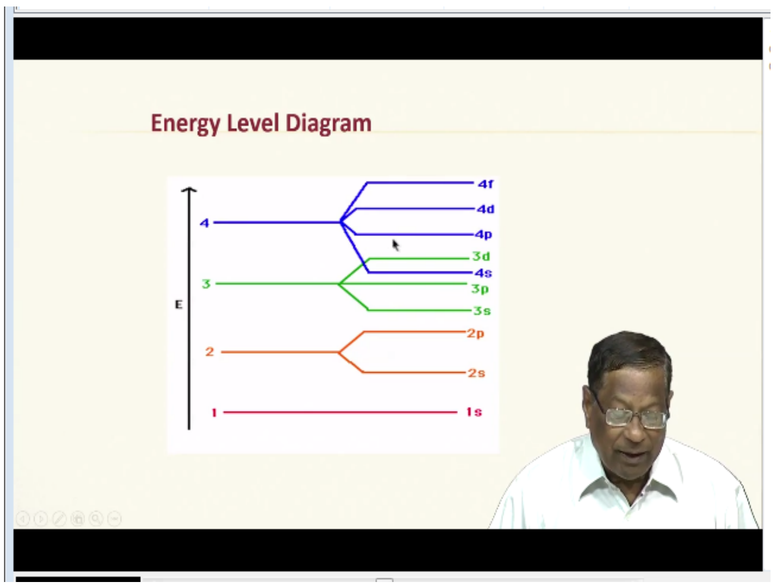

And then d this is the energy level diagram of the electrons in which the filling of the electrons takes place for as the atomic number goes up. Here I have 1, 2, 3, 4 something like principle quantum number equivalent to that. And this is the energy and the energy of 1s electron would be very less there will be 2 electrons in this. And there are no p or other orbitals here around 1s, 1p etc. 1p there.

Because l is 0 for l=n-1, so that is 0. So, there are no p orbitals or any other orbitals similarly for second principle quantum number we have 2s and 2p that is the 2p orbitals there are 3 2px, 2py, 2pz. And then similarly if I as I go up I have 3s, 3px, 3py, 3pz and then 3d orbitals but if you look at the energy level diagram you can see that 4s is slightly lower than 3d orbitals okay. So, the energy of the electrons that are resigned in 4s is lower than 3d.

So, this is again sort of but it is there all the time. And then I have 4s 4p, 4d, 4f electrons. And then 5s, 5p, 5p, 5d etc. as the electron filling takes place okay.

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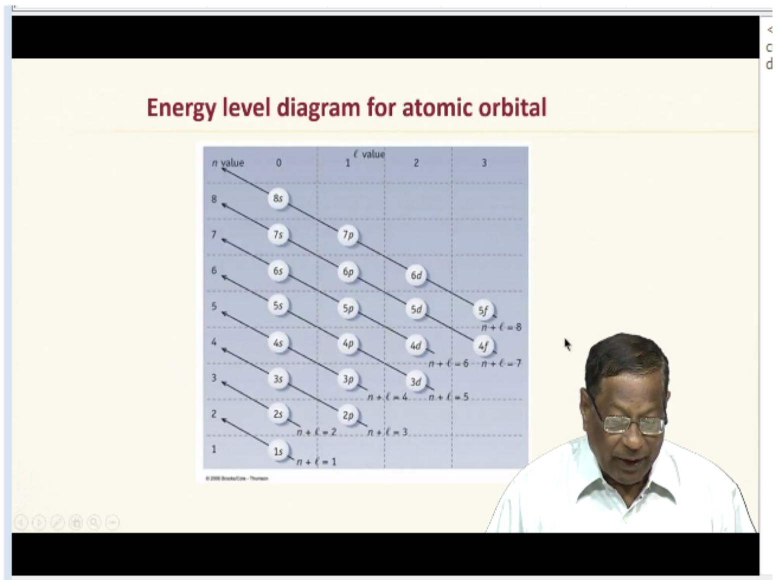

Now the energy level diagram of the electrons can be visualize like this here, I have principle quantum number n here. So, I have 0, 1, 2, 3 etc… l values are here. And then the principle quantum number 1, 2, 3, 4, 5 up to 8 I have given okay. And then I have 1s the energy of the electrons in n+l it is varies from this level to this level. So, 2s would be varying up to this level up that is up to 3s okay.

So, like that here I have n+l=2 and n+l=3 okay. So, I have similar arrangement here this another way of looking at the felling of the electrons or energy level diagram that is prevalent in the atomic structure. Okay.

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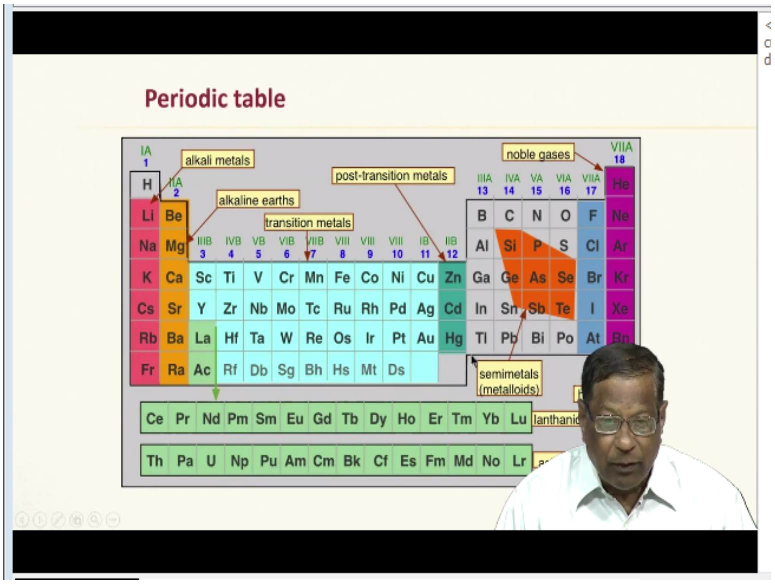

Now if I go on doing this that is if I keep on filling the electrons 2-2 electrons in each orbital. I have a number of I will be constructing theoretically a number of elements with 1 electron, 2 electron etc. And the all those electrons can all those elements can be arranged in the periodic table. I am not going to describe spend much time on this because this information is required only for the understanding of the atomic structure rather and in relation to infrared spectroscopy.

I am giving you the final form of the periodic table as we understand it today, actually there is a lot of there are lot of experiments, lot of hot burns, lot of research lot of time. You know in terms of years together have been spent in organizing the number of elements that we know into a short of periodic table. And that itself is a matter for another lecture or only on periodic tables but I have we are going to skip it little bit.

But suffice it to say that all the elements in the as you know them today are can be arranged in terms of their increasing atomic numbers. And atomic number is the fundamental property of the element of any element and starting from hydrogen with least number of atomic number and number of electrons we have up to lawrencium almost 108 or dysprosium is also there, lawrencium is the actinide series that is the last element.

And we have up to this element, so all these elements can be organized in this fashion and there all arranged in rows and then vertical columns and then I have separate transition elements here and the I have different kind of triodes here, zinc, cadmium, mercury and there is another triode here silicon, phosphorous, selenium or germanium etc. All these elements these arrangements have got significance.

Because significance of properties similar properties because they have as the, so they have been arranged in different colors. So, for example hydrogen here after hydrogen next element should be here where it is written as s2A. But it is not there next element is helium and the next element is third atomic number is lithium, beryllium. And then there is a big gap here it is only convenience as far as we are concern.

But lithium, beryllium, boron carbon, nitrogen, oxygen, fluorine and neon are second group elements and then similarly I have third group, fourth group, fifth group, sixth group etc. And the left side elements lithium, sodium, potassium, cesium**,** cambium etc. These are all alkali metals these orange colored once beryllium, magnesium, calcium, strontium barium and radon radium. There all the alkaline earth metals.

And the once in this the blue color, green color there all transition metal elements. And I have coinage metals here ion, cobalt, nickel Ru, Rh, pd. And then copper also to that to some extent osmium, Ir, pt this is another triode here which similar properties. And then I have lanthanum and actinium, these 2 are marked differently colored. Because here 3d and 4d, 3f and 4f, 4f and 5f electrons getting filled up here that is inner electrons.

So, this constituents from 51 to 72 that is up to lutetium will be here. So, all these elements exhibit similar properties because the electron goes into in inner orbital. So thorium protactinium and uranium and all these things these are all actinides and many of them are radioactive elements etc. And once we come to this area you can see the arrow pointing here these are all sort of non-metals boron, carbon, nitrogen, oxygen etc. And these are all metalloids and then I do have certain amount of metals here aluminum, gallium, indium, lead, bismuth etc.

And then I have halogens here fluoride fluorine, chlorine, bromine, iodine etc. all the almost all the elements are covered here in the periodic table. This sees our understanding of the periodic table as of now okay.

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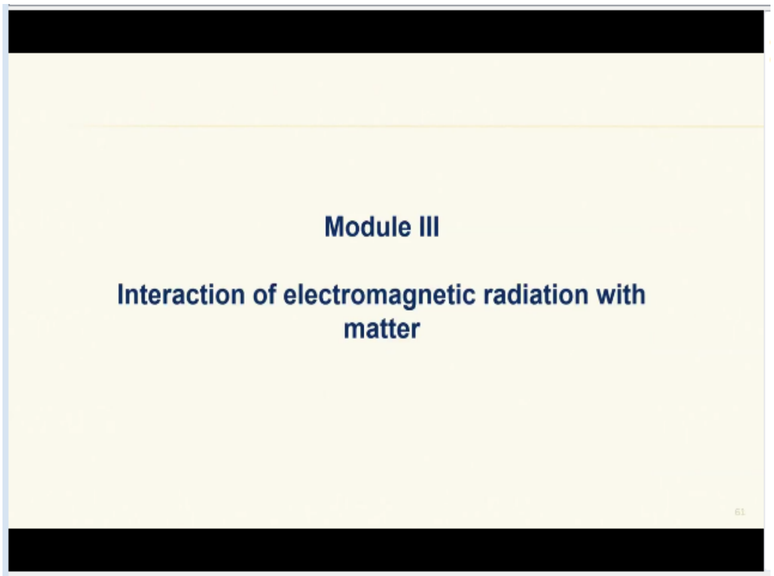

So, what I wanted you to understand is that the periodic table as we understand today is based upon the electronic structure of the atom. And then the periodic table is arranged according to their properties and among the periodic table I have the element carbon. And carbon is a special element as you all know we all know because carbon has got a capacity to bond itself to other carbon atoms as well as many other elements like hydrogen, oxygen and then nitrogen, phosphorous many other elements.

So, this study of organic compounds itself is a separate specialization by itself known as organic chemistry many of you know it. And our course depends our course is actually the pollution monitoring of the organic compounds. Because infrared spectroscopy mainly deals with this spectrum of the organic compounds, so before we proceed on the infrared spectroscopy details what I would like to do is I will take you to the next module that is the electromagnetic radiations and it is properties okay.

So, my next slide shows you the module that is Interaction of electromagnetic radiation with matter we have finish the introduction part of this course. And now we are going to talk about the electromagnetic radiation.

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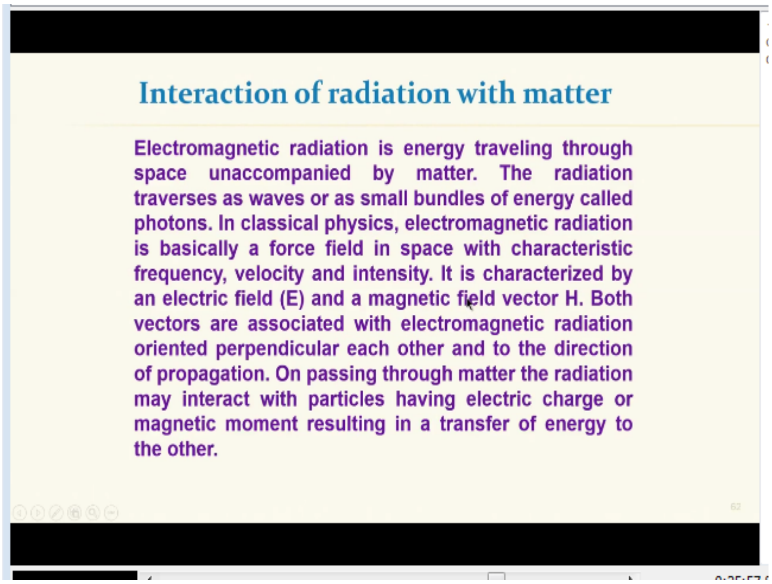

So, what is electromagnetic radiation I want you to understand that the electromagnetic radiation is energy travelling through the space unaccompanied by the matter that is the basic definition of the electromagnetic radiation that means as you and I sit here in front of each other or TV or something like that. There is electromagnetic radiation flowing around all of as in between the space between you and the computer between me and the computer and in the room outside the room everywhere electromagnetic radiation is around us.

So, you have to understand that, so but it is sometimes visible sometimes it is not visible. So, the how is what is this electromagnetic radiation that is the fundamental question. So, it is the some form of energy that is flowing all around us and we are also part of the system okay, so this electromagnetic radiation as said it is flowing around that means it keeps on moving okay. So, as the radiation moves or as the radiation traverses is it is it traverses is as waves or is small **of** bundles of energy.

They are called as photons okay and these in classical physics the electromagnetic radiation is basically a force field in space with characteristic frequency, velocity and intensity. So, an electromagnetic radiation can be described as having 3 properties one is the velocity it has a frequency and it has intensity. And this is the part of the electro part and parcel of electromagnetic radiation.

Every electromagnetic radiation if you try to understand what is electromagnetic radiation definition apart what else is electro what you understand by the electromagnetic rad by the term electromagnetic radiation it may be in the form of light blue color, white color light etc… sunlight, moonlight and then dark light radio waves energy waves, micro waves. In our kitchen and all you use micro waves and all these kinds of energy forms can be described as electromagnetic radiation okay.

Now it is very clear that we do not see the electromagnetic radiation around us all the time we see only a small part. Because whatever is visible to our naked eye we see that we see orange colored light, yellow color light, red color most of them we describe by VIBGYOR that is rainbow colors violet, indigo, blue, yellow, green, red and where white you know all those colors.

And just like in rainbow we find all the radiations that are visible to our naked eye are the electromagnetic radiation that is experienced by us with our only with our eye contact. Then we experience other electromagnetic radiations also around us sometimes even if it is at night we feel hot. And then there are other ways of looking at it in micro waves etc. We cook at homes, so it is the how do you describe an electromagnetic radiation, we do describe electromagnetic radiation by the common properties what every electromagnetic radiation should possess okay.

So, what are those properties those properties I have already told you their frequency, velocity, and intensity. So an electromagnetic field is as it is names suggest it has an electric force field and a magnetic force field. Both these are vectors electric field and magnetic field vectors do you know what is vectors for those of you who do not know what is vector, vector is a direction oriented force field with magnitude.

So, when I want to represent a vector I show the direction in which the vector is there. And also the quantity of the vector, so you can read up a little bit on the fundamentals of electro fundamentals of electromagnetic radiation. You will immediately come to understand much more than what I am trying to tell you about the force field vectors. So, both vectors are associated with the electromagnetic radiation.

They are oriented perpendicular to each other that means I have whenever I describe an electromagnetic field. I have 2 fields associated with each electromagnetic radiation one is magnetic another is electrical electric field. And these fields you can feel the effect of the electro magnetism and electricity along with each other. But they have aligned perpendicular to each other and to the direction of propagation.

So, on passing through the matter the gain I am going little bit abstract here when an electro radiation passes through the room in which I am sitting or in which you are sitting. There is the interaction between the electromagnetic radiation and matter takes place. So what is a matter, so matter could be empty space it could be the particles in the room in through which the electrons through which the electromagnetic radiation passes or it can pass through a last piece or it can pass the cut while trying to pass through a door or a wall or anything.

But electromagnetic radiation is always there, so much so that even when you are sitting in a closed room which is totally dark there is what is known as there is dark current dark electromagnetic field is there some that is known as stray light. So, the stray light is again another concept of the instrumentation in the electromagnetic radiation that is in our concentration also with respect to infrared spectroscopy.

So, you will talk about stray light later, so on passing through the matter the radiation may interact with the empty space with the particles or with the molecules of air that are present in between you and we or wherever it passé through it has to something has to be there either empty space or they particulates or the gas molecules or vacuum empty space means vacuum. So, any of these things are there, so the electromagnetic radiation interacts with the matter okay.

And when the interact the electrical charge and magnetic moment they get transfer to each other from the matter to the electromagnetic radiation or from the electromagnetic radiation to the matter. So that results in a transfer of energy to the other, so that is the interaction of electromagnetic radiation with matter.

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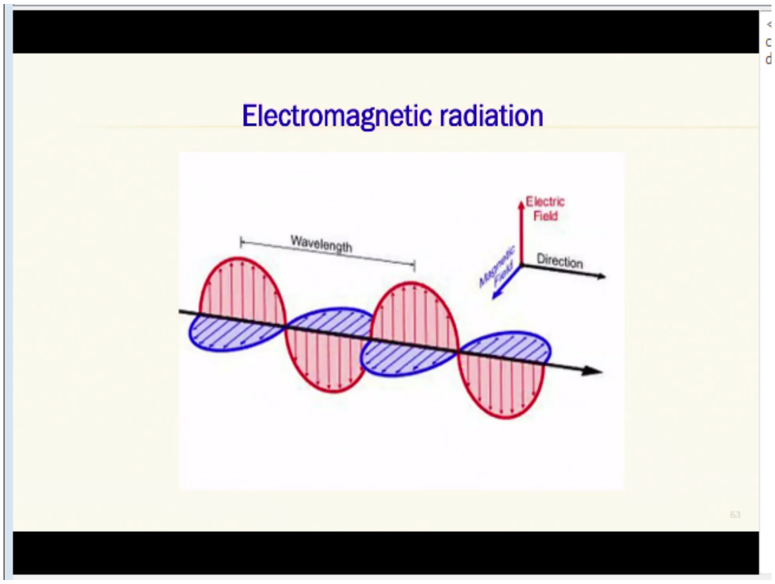

And we will continue our discussion in the next class more about it later, thank you.