Theory of Group for Physics Applications
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Lecture – 13
Point Group Notation & Factor Group – I

So, called Schonflies classification, but as I was looking at this I admired the size of this group is called the largest group.

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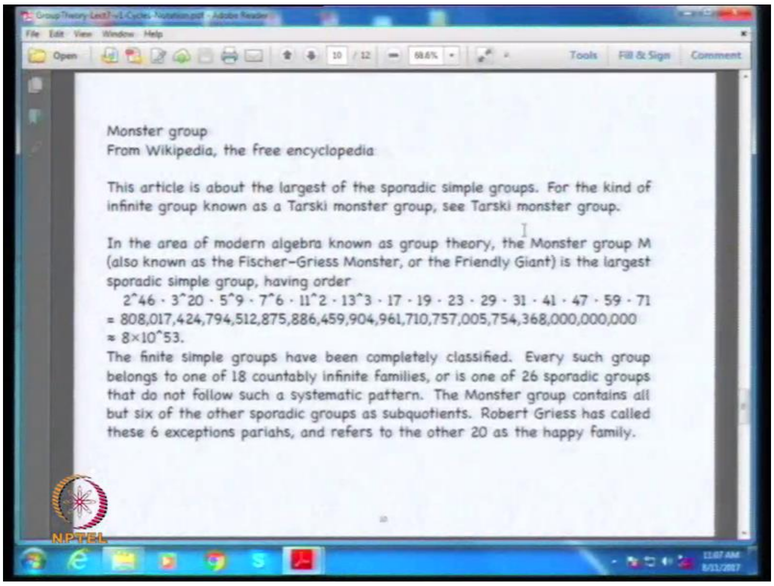

Well the largest of the exceptional groups because there are infinite ones which are classified like the cyclic group of prime order. So, those are of course, there, but if you look at this is so, this actually also tells you perhaps the cycle structure 2^{46}, 3^{20}, 5^{9}. So, it is some number, but the thing to remember is that even this is embedded in a symmetric group, in a permutation group whose size is this many factorial.

So, even this group is embedded somewhere in some symmetric group; so, that is nice to know. So, by the way I have been reading quite a lot about this because not about this particular thing, but group theory to teach you have been studying a lot and I am realizing that in the last 25 years or so, there has been such great flowering of this whole technique; not that group theory was not known, group theory was known to mathematicians for long time.

The theorem they are all from 19th century, but it at its application in physics was just taking off in the 1960, 70s which infrared spectroscopy, Raman spectroscopy some few rudimentary you know spectroscopies, but in just the last 25, 30 years it is really have undergone an exponential growth in the techniques that can detect all kinds and the material science has grown.

So, all these methods where they being applied to physics and to chemistry and the other thing is I hope no chemists mind by saying this, but when we were learning chemistry it was all about you know colors, smell and what mineral it comes from and all this. But now, chemistry has actually become a physical science with understanding in terms of the molecular bonds and which ultimately boils down to quantum mechanics and symmetry. So, that kind of understanding of chemistry has also grown by leaps and bounds.

So, there are lots of sources now available which clarify all of this quite well. So, that is why I am probably finding it difficult to teach all of this because suddenly that has been such a great growth lot of things I did not know have come around.

And so I hope that you will understand that although it sounds like a very old subject, it is really from the physics and the sciences point of view; it is the subject under growing a great growth still lot of things are happening in it. And you may know the story of DNA discovery where this was 1953 or so; the two physicists Crick and Watson. The biologists were taking the X-ray crystallography of the molecules and storing them and trying to study them.

But Crick and Watson kind of spied on somebody else's lab, biologist lab understood that the crystallograph represented the double helix. I think the crucial thing was also the hydrogen bond between the spirals and they understood the presence of all this and they were able to crack the code.

So, ever since then X-ray crystallography is very very important also to all the biological sciences. So, all of this is growing very rapidly and we will just try to do the basics and the basic ideas of how it can be applied. So, towards that we will focus more on the molecular groups.

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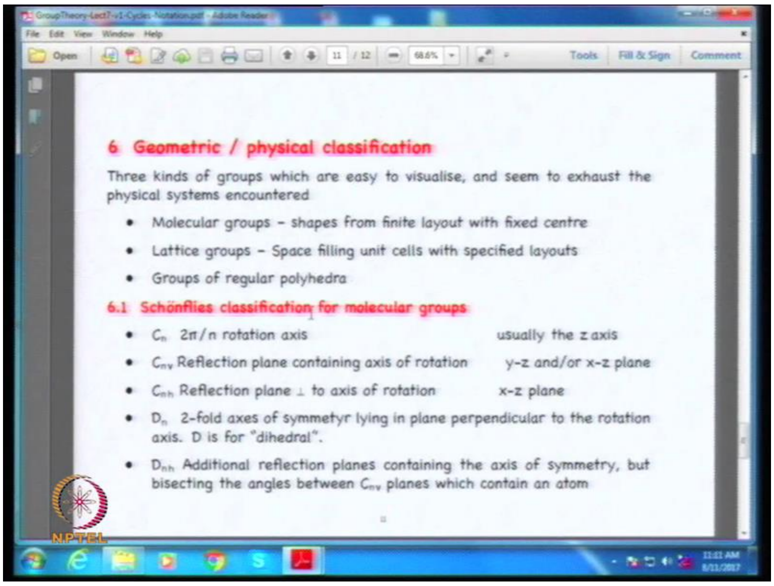

And what is Schonflies classification? Schonflies is also from turn off 1900s from; 1800 something to 1900, but this is the notation known after him and then there is another one which is used for crystallography.

So, we will not get into that because to get into it you have to actually start understanding crystals and start understanding other physical effects which are not part of this course. So, to just illustrate how does mathematics can be used we will applied to the simplest and more obvious systems. So, to begin with this classification, there are three broad categories in which the group theory is applied; one is the molecular groups, where there are shapes of finite size with the fix centre and the other are lattice groups which are space filling.

But you try to map out of the symmetries of the unit cell, but the translation in variance goes with it. So, the entire group of symmetry is actually consists of the product of both the and the translations are also along fix lattice directions. So, those lattice vector translations and also there are some screw shift symmetries and so on. It gets much more complicated and interesting if you are studying those systems, but we will confine. One thing I want to mention here among the lattice groups.

So, it turns out that because of this fact of having to have translation invariance; the symmetries of the unit cell have to be such that they are compatible with translations. So, they have to be space filling, so this puts a restriction on the number of groups you can have, number of molecular kind of groups you can have in a lattice. So, for example, in the plane; you can only have 2 fold, 4 fold or 6 fold symmetry.

Because with a square or a hexagon you can fill the 2 dimensional plane, but with say pentagon; you cannot really be I mean that is what people thought you cannot be filling the space and with other shapes you cannot. A surprising discovery in the 1960s was that actually there were crystallographic that showed pentagonal symmetry in a space filling way.

And everybody thought that the guy was the cracked pot; eventually got noble prize about 5 years ago for discovering this. And the solution was that the pentagonal symmetry existed, but there was no translation invariance really, there was approximate translation invariance you cannot really fill in a symmetrical way.

So, actually it is never repeating patterns in the sense, if you just kept extending it you can keep filling the space where every one of the nodes will have pentagonal symmetry around it, but the pattern as a whole does not have translation symmetry; has approximate translation vectors which have to be kept modifying as you go further away. So, that was a very interesting discovery of a group that is not quite a lattice group, but it is a space filling pentagonal symmetry and apparently it was there in M C Escher's; you know M C Escher's painting Escher; you should look up M C Escher's graphic card, so some of the space filling pentagonal thing are there in it, but they do not become there is no translation invariance in 5 directions as such. So, now as far as this let me actually switch here for a moment.

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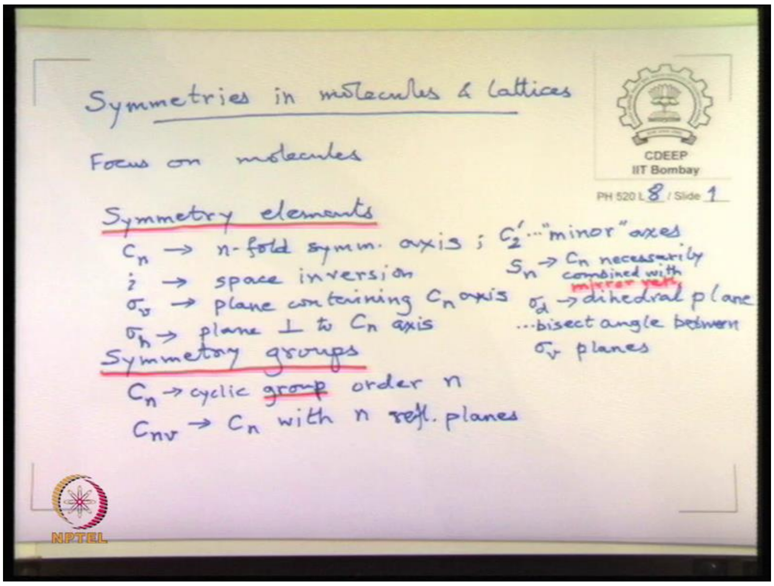

I was about to say symmetries in physical systems, but that would be too vast. So, molecules and lattices and we will specifically focus on molecules. So, here I want to say something that I found in that is kind of missing in many textbooks which most diligent student will learn without being told, but because I like to say things more clearly.

There is a redundancy of notation, there is a set of symbol for symmetry elements and then there is a set of symbols for symmetry groups by C_n, they mean n for symmetry axis, no surprise. Then there were symbol i which is space inversion where you send each of the 3 axis into negative of themselves $x \rightarrow -x$, $y \rightarrow -y$, $z \rightarrow -z$. And then there are symmetry elements called σ_v; so, σ is referred to some planes usually. So, C refers to axis, σ refers to a plane.

This typically a plane that contains the C_n axis and then there are σ_hs horizontal set which is usually perpendicular to the C_n axis. There are couple of more things, there is also σ_d dihedral plane; we are just within the writing which usually bisects two of the C_v planes; bisect the angle between σ_v planes; I am sorry. There will be this notation C_2' or C_n'; usually only C_2' which are some kind of supplementary axis they are not like the main z axis, but axis that are perpendicular to it.

So, if you think of benzene you have 6 fold symmetry axis passing through the center, but then through in the plane you have 3 axis is available around which you can flip the whole molecule the plane turn it around usually a C_2 axis, but they put a prime on it just to show other it is minor one, it is not the major one.

So, less important not minor in any other sense; finally, I am sorry I have packed it up like this, but maybe it is now becoming a two column format. There is something called S_n which is C_n necessarily combine within improper rotation, C_n combine with mirror reflection. So, this when you have staggered configuration; I will show you we will come to this combined with what they called improper rotation; so, it is a mirror reflection.

So, that is about symmetry elements now you will find that there are various group listed by identifying these element. So, you take a molecule and then you say does it have a C_n, does it have a C_h, does it have a σ_h, does it have a σ_v? etcetera, then you decide oh yes my group is C_n; it is a same symbol used, but now it is meant to denote the group. It is essential that cyclic group of order n then you designate things called C_v; C_{nv} that is C_n with n symmetry planes and reflection planes containing the axis. So, this we had written somewhere is not it.

So, here you can see we have written down that classification for the molecular groups. The C_n groups are with a redundancy of notation; C_n groups are those that contain a C_n axis. So, C_n basically has 2π/n fold axis of rotation usually it is denoted the z axis.

And most books just assume it is it has be z and what else it can be; then C_{nv} is the set of groups class of groups which have C_n rotation axis that is 2π/n rotation axis and reflection planes containing the axis of rotation. These are yz and or xz plane; these are planes that will usually contains z axis definitely because it is itself σ_v element which contains that axis could be yz and zx, it could be even other planes. Then C_{nh} are things with this 2π and rotation axis, but a reflection plane perpendicular to axis of rotation.

So, it has same structure above and below; we will see some examples of this. In this case it is since it is perpendicular to the axis of rotation; it should be xy plane not xz; this is the error I have to correct. Then come the class of things called D_n and the D_n are essentially molecules that help 2 fold symmetry in the plane perpendicular to the axis of rotation. So, maybe I will come to the pictures right away, we just finish saying this and then we will see D is for dihedral and then additional D_{nh} are additionally reflection planes that contains axis of symmetry, but which also have planes bisecting angle.

So, they have this element σ_v as well as σ_d. So, we will come to this and there is S_n which include the improper rotation. So, the same symbol S_n is used for a group element as for the group entirely that consists only of S_n's and when writing S_n, it is emphasize repeatedly if it is possible to get away with n fold rotation alone without reflection, then it has to be called C_n. These are special things where you rotate, but there is a staggered symmetry so, that after rotating you must also reflect to recover the molecule.

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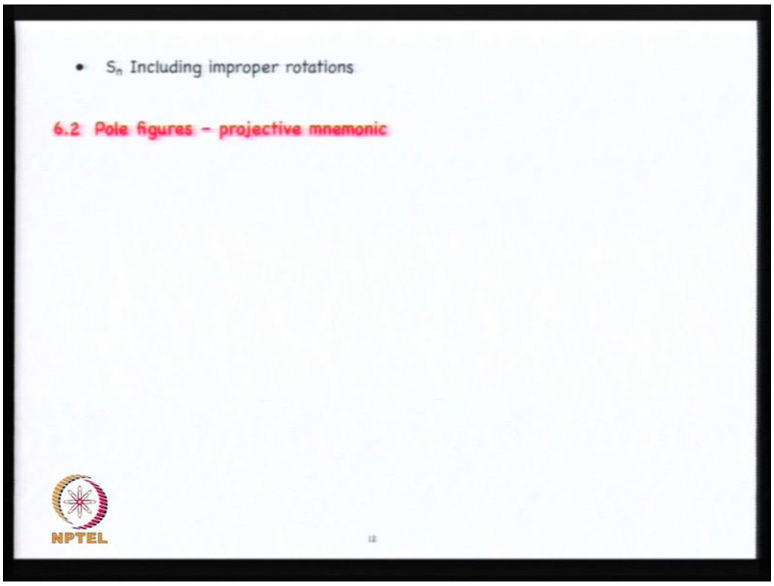

So, we will see the examples now and for this I have downloaded a nice presentation from German University.

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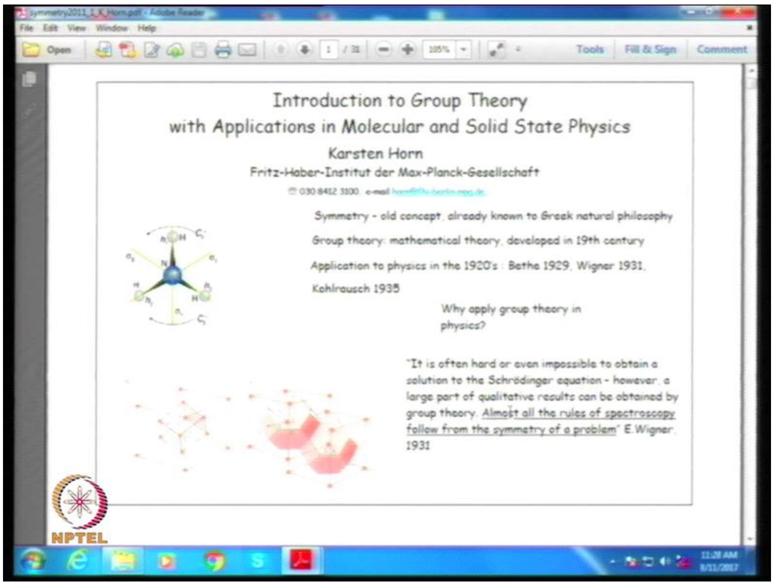

So, this is as you see 31 slide PDF, but actually each slide contains two of it is PPT slide; it is about 60 plus slides and it is a complete crash course on everything we are going to do not everything, but most of it.

So, since it is an opportunity to go over some of the more important things let me just show that. So, he has quoted using Wigner who was one of the pioneers applying group theory to physics including molecular symmetry, relativistic invariance everywhere Wigner worked out the symmetric groups and their representations and etcetera.

And Wigner also seems to have remark that some point that this is unreasonable applicability of mathematics to physics. That so, much physics would be explicated by application of 19th century mathematics was completely unexpected. So, it calls group theory the unexpected applicability of mathematics to physics.

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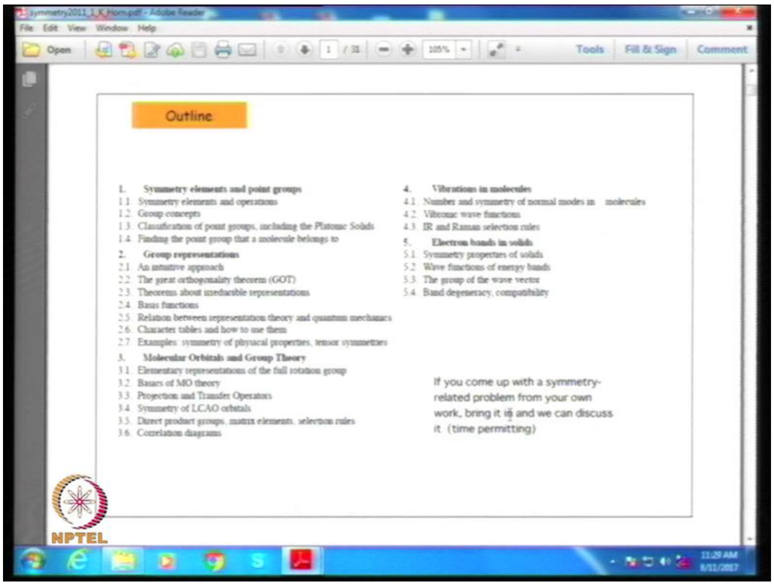

So, here is the list of this thing.

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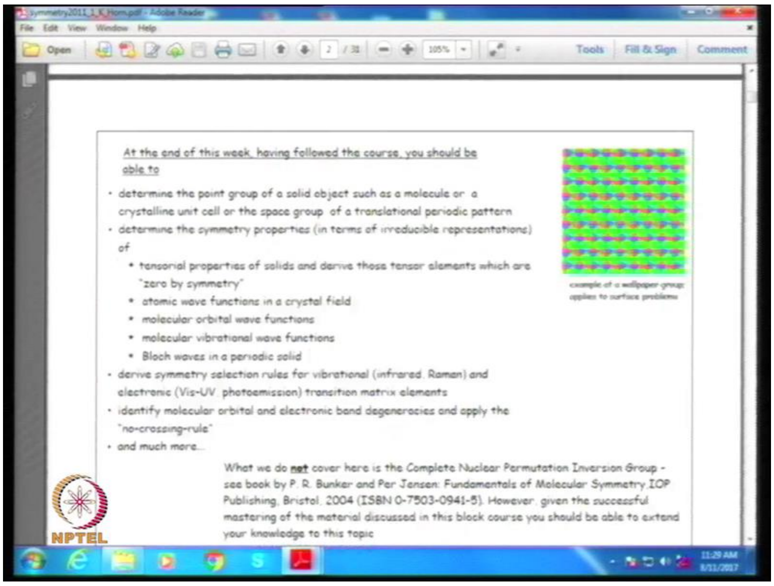

This is a space filling group but this has translation invariance as well, but there is additionally colouring. So, it is called from wallpaper group we are not going to do that.

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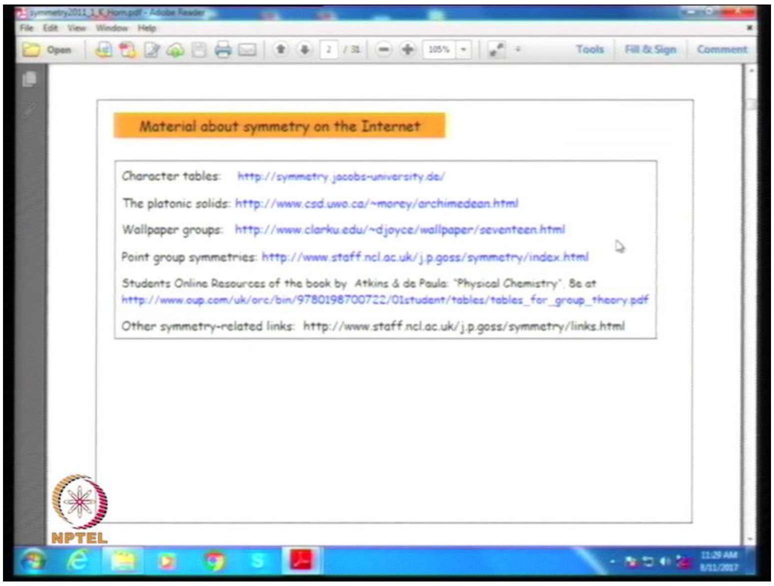

He has given the various kinds of links to outside sources; so, you do not have to judge me because he also used the link; so, I use his link.

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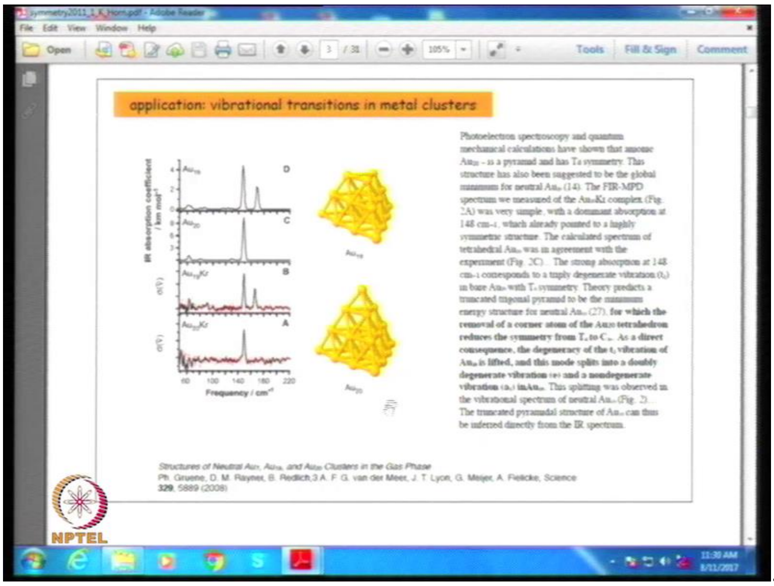

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This is a nice example of what we are not going to do and since we are not going to do I may as well show this transparency nicely. You can read all this text because I will put it up or give a link to this, but main point is they have now discovered a gold 20 configuration; 20 atoms of gold form themselves into a little pyramid like this.

And so, here is the Raman spectrum corresponding to it and because of the high degree of symmetry, you get a very sharp peak because there is a huge degeneracy of levels that do this. And here to show off they have that theoretical calculations which exactly match it and then you create of course, it is done there is some detail you are the same Krypton added to stabilize it or something like that, but apparently does not affect the symmetry.

Then they work out, they claim that actually energetically more favorable is gold 19, not gold 20; where you chop of this top and then you are left with a truncated pyramid when you truncate it; the degeneracy of these levels breaks and some of the levels shift in frequency.

So, you get a shift in the frequency actually here these are the ones with red dots are the experimental data. And they get a peak over here there which they are able to reproduce exactly if they assume that this is what happened. So, symmetry can be used to exactly fit the end you can get the relative height of the peaks from this as well, from group theory as well because the multiplicity of levels that will give this transition versus this that ratio will be the ratio of the at least the amplitudes of this, if not the intensity ok; so, that is one of the uses.

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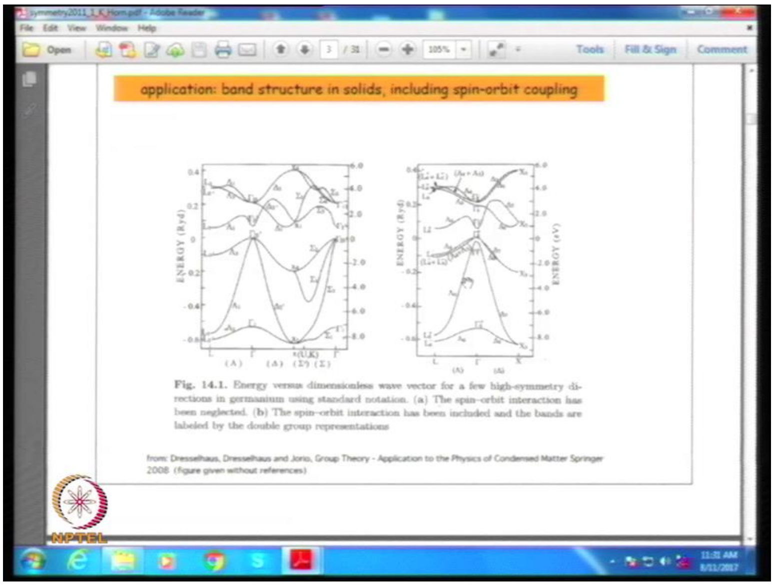

And similarly here this diagram is bit difficult to look at it first, but roughly speaking what it shows is that whether you include certain symmetries or not, let me leave it at that. But you can see a coincidence of this is from condensed matter physics; the x-axis the y-axis is energy in the red berg of the level; it is a band structure and the band is dependent on the momentum vector the wave vector k, wave number vector.

So, x-axis is wave number vector and there is a unit lattice. So, that k has a finite length I mean the values; there is a particular one where there is a coincidence of lot of levels coming together and that also has to do with group theory and you can deduce it from the group embedding of that unit cell the symmetry of that unit cell.

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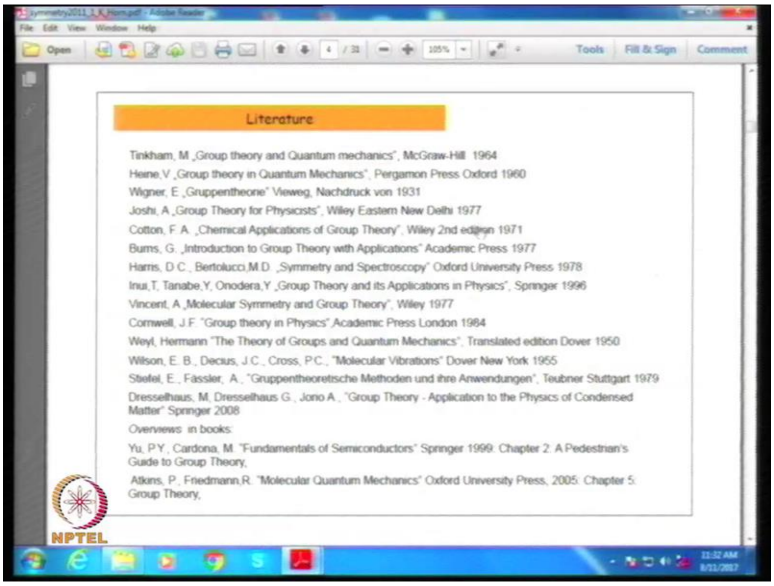

So, there is long list of literature.

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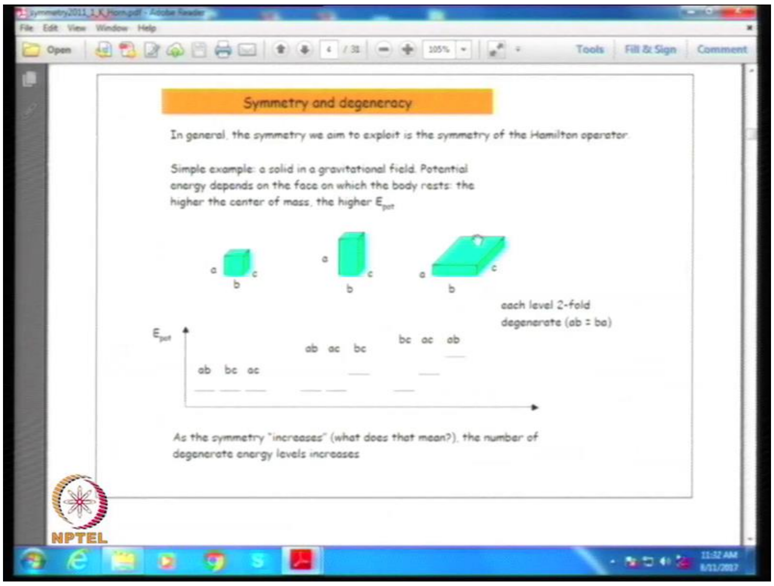

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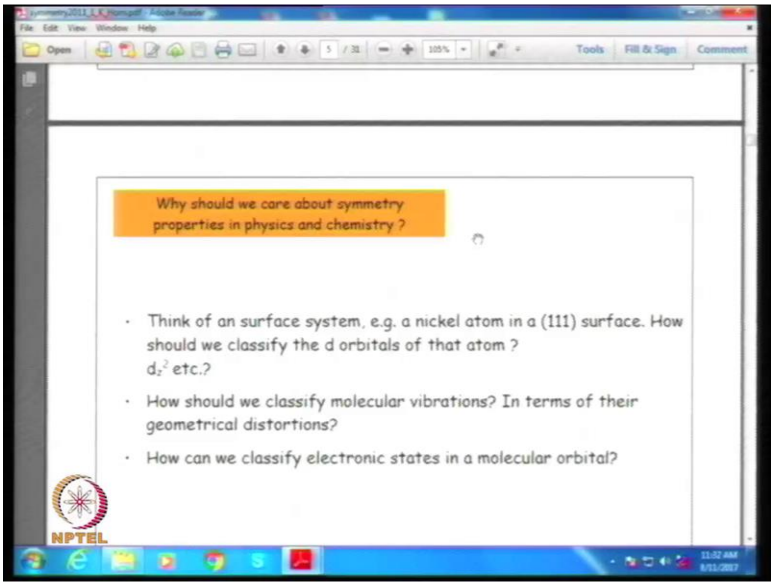

Then there is early part of the group theory discussion which you can for revision if you like, but I want to focus on yes classification of point groups.

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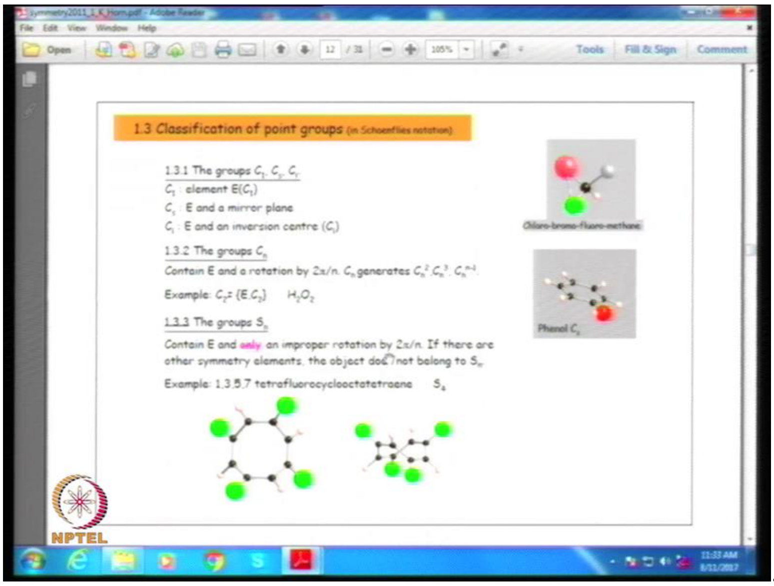

So, begins with saying there are groups C_1, C_s and C_I as I said there is going to be a redundancy in what is meant by an element of the symmetry operations and a whole group. So, C_1 even basically has no symmetries and C_S essentially has only a mirror plane and nothing else. So, I think in this example, this has no symmetry that all I think this is C_1 and then there is mirror plane which exists in the case of this molecule because it is planer, but it has no the rotational symmetry is because of this red thing add on then we come to there is this 3 categories of and C_I; I is the inversion element. So, space inversion is included, but there is nothing else possible.

So, that is these are the simplest very trivial groups this is this is only 1 element and these two have 2 elements each then we come to the bigger groups. So, C_n and as we have been saying contain the identity element and the $2\pi/n$ rotation axis. So, you can understand what I was trying to tell you the group is called C_n, but then here this C_n means this C_n axis ok. And the C_n axis one rotation squared gives you C_n^2 , C_n^3 and C_n^{n-1} these are n fold rotations.

So, these are elements of that symmetry raised to power n you will return to E. So, C_n group will contain C_n axis sorry for the redundancy that C_n axis rotation done n times brings you back to identity. So, this line the C_n refers to the group element here it refers to the group itself. And the example that here as chosen is H_2O_2 hydrogen peroxide it is not shown here, it is a non planar molecule.

So, you can rotate it 2 fold only it like an arm chair. Now, come the S_n group which is what I was telling you have to be careful contains E and only an improper rotation; if it contains proper rotations usual C_n rotations then you have to classified with this other classifications.

Those things that have identity element and only improper rotations by $2\pi/n$ are called S_n and you can imagine that axis is called as S_n axis. And the example is this tetraflurocyclooctatetroene ok. I said it if you look at this picture a little carefully what it is trying to shows that this green and this green are coming out of the plane and this green and this green are dip below the plane.

So, there is this octagonal planer system and then these 2 greens are attached to it coming out of the plane and these two are attached going into the plane. And similarly 2 of the whites come out of the plane and 2 of the whites go into the plane. And that thing is shown inside view over here, but it is not also immediately very clear, but that is what 2 of the greens come out the ones that are opposite; they come out of the plane into of the greens go below the plane similarly 2 whites are out and.

So, now, you can see that I can rotate this group by this molecule by 90 degrees that will bring this green over here, but it will still be about the plane.

So, to get to the original configuration how to flip it in the plane containing the octagonal ring; so, this is exactly an example of an S_4. So, this is good example and incidentally from reading other translate and read lots of them reading another transparency I know that in fact, this comes in two configuration this is called boat and there is another one where this these two are flipped up and down and it is called a chair.

So, there too nearby ones will be above too nearby ones will be below that become like an arm chair this is where they are like this in this called boat ok.

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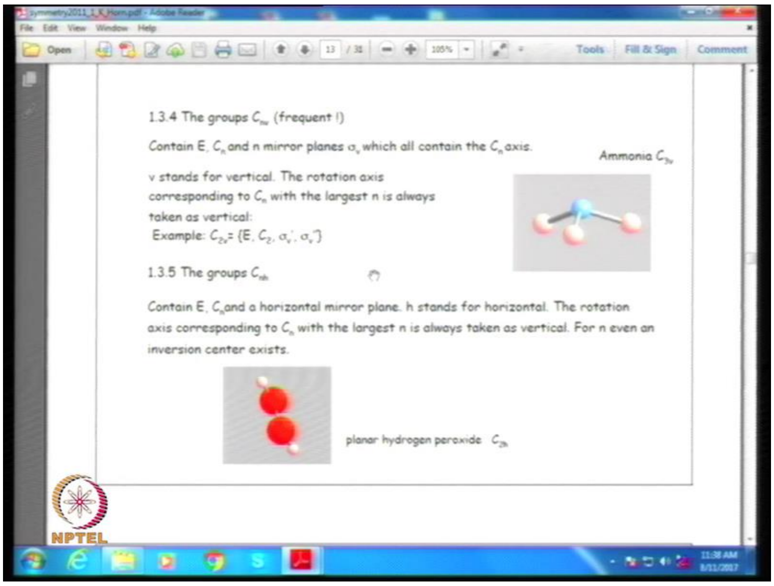

Now, we come to this nomenclature C_{nv} which is very frequent as it says it contains identities C_n and n mirror planes σ_v. So, σ_v are planes which contain the C_n axis the simplest is this ammonia molecule where you of course, have this axis vertically about which you can rotate $2\pi/3$ at a time.

But then you can draw a plane which passes one of the hydrogens and then the nitrogen or this hydrogen in this nitrogen or the this hydrogen in this nitrogen. In fact, I called them $\sigma_v{}'$ and $\sigma_v{}''$ axis the one containing identities probably left out. So, again this primes are used just to indicate that they are somewhat of less important elements or that there is a multiplicity of them.

So, this is C_{3v} and it would contain $\sigma_v{}'$, $\sigma_v{}''$ and $\sigma_v{}'''$.

So, should not be left out then there are the C_{nh} groups which contains C_n. So, it contains this, but h means a σ_h plane horizontal plane horizontal plane. The rotation axis corresponding to C_n with largest n is always taken as vertical. So, z-axis vertical is; obviously, z right for n even n inversion center also exists. So, here there is a; so, this is the hydrogen peroxide molecule no this is not hydrogen peroxide molecule no it is written plane; so, this is the planer version.

But on Wikipedia when I read hydrogen peroxide it said both in gaseous and in crystalline form; it is essential a non planer molecule. Anyway we can take this whatever is drawn here for the time being where this pink ones which are hydrogen and big red ones which are oxygen all in one plane, but they are staggered this is here that goes back, then this red comes forward and pink goes back. You can see that this has a σ_2 plane, you can rotate it by σ_2, but it does not contain a vertical symmetry axis right. So, the z axis in this case runs like this it run perpendicular to the plane of the molecule.

You can do a σ_2 rotation, but there is no C_{2v} plane because there is no symmetry plane passing through to this axis; however, there is a plane containing the whole molecule which is a horizontal σ_h plane and that is for it would be σ_{2h}.

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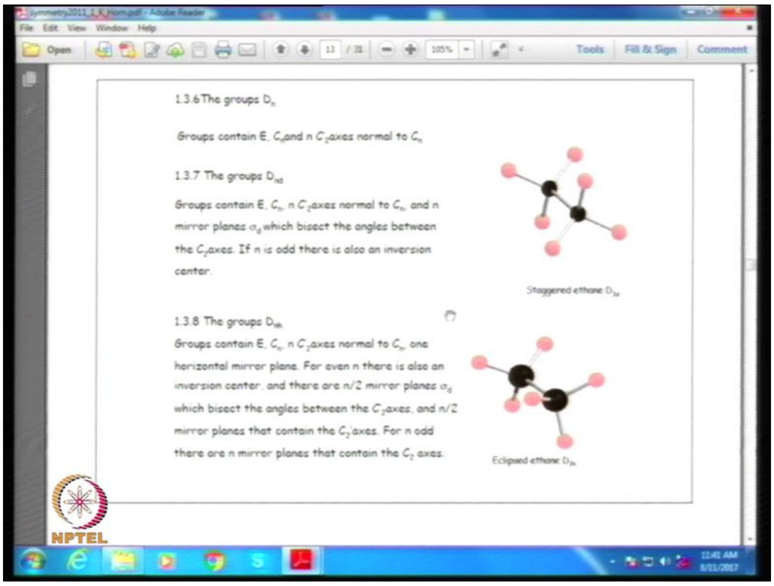

In fact, if you go that site water bind it will show all this along with animations ok. So, then the group is D_n; So, D_n contain E, C_n and then there is a prime which is not visible here n number of C_2'. So, n number of C_2' axis which are normal to the C_n.

So, this is a 3 this is a D_n; but with the D there is no simple example of a D_n given, but you get the idea well you can just think of a cube then it has 4 fold symmetry axis. And then the plane perpendicular to this axis contains at least 1, 2, 3 and 4 perpendicular to it where you can flip the whole. So, do not let make it parallelepiped; so, that there is no other symmetry. So, there are 2 squares and there is a long side to it box like this, but you can flip the whole box by an 180 degrees, but there are 1, 2, 3 and 4 independent axis available for flipping.

So, that would become a D_4; it would have C_4 and 4 C_2' axis perpendicular to the C_4 that would make a D_4 group. Then the D_n group which contains this C_2' axis and mirror plane σ_d which bisect the angles between the C_2' axes. So, this prime is missing here which bisect the angle between the C_2' axes; if n is odd then there is also an inversion center.

So, we can look at this molecule which has triangular configuration like this, which is not planer by the way. Although these 3 are in a plane the black one is not in the same plane as these pink ones; there is back further back is black one and then there are 3 pink one which are again out of that plane, but the 3 pink ones are in a plane.

Now, if you compare the location of this triangle with the triangle in the back; the 2 triangles are staggered by 30 degrees. So, that this apex if you project in downward will fall in between these; so, this satisfies these criteria that you have. Firstly, drawing z axis through this you have a threefold symmetry because you can keep rotating this one which will come back to itself.

You do have n number of C_2 axis is normal to C_n; you can draw an axis passing through I mean along say this pink and this black direction, this pink and this black and this pink and this black; those are equivalent to drawing also through this pink or this black.

So, there are 3 independent axis which are perpendicular to the z axis around which you can 120 degree rotation and you will know that actually it will not come back to itself; it this will come in a staggered position d and σ_d right. So, this is your n C_2' axis this is normal to C_n this does not have that because a 120 degree 180 rotation will bring this pink to a staggered position here. So, I have a problem with this ok.

In any case the if it is meant to give the example of dihedral plane that is what is the important thing. So, we draw these C_2 axis which are perpendicular in between them are;

so, there is a reflection plane which contains the z axis and which bisects this axis and this the rotation axis about this and rotation axis about this; isn't this correct that those axis are not C_2 axis.

But there is certainly a dihedral plane which is in between these two which is a symmetry. So, there is a dihedral plane that bisects the angle between the C_2 axis and then D_{nh} these contain E and there is if n is odd there is also an inversion centre. Because you can see that if you are sitting in the centre of this rod which is the z axis symmetry axis and if you do a space in version, this pink will going to that pink and this pink will get flipped into that pink.

So, there is a space in version symmetry present whenever you have odd number of these then D_{nh} ; h obviously, means there is some σ_h plane. So, it contains e, C_n, n $C_2^{'}$ axis normal to C_n and one horizontal mirror plane for even and there is also an inversion centre and then there are n/2 mirror planes σ_d which bisects the angles between the $C_2^{'}$. So, this is a little better the so, called eclipse ethane these pinks are in corresponding positions ok.

So, if I flip I have a mirror plane and if I flipped I will get this to go to that this to go to that that; so, this is quite clear, it actually fits the our this criteria the. So, forget the D right now; so, C_{nh} and then there are mirror planes passing through this pink and this pink and the 2 blacks which will be extending like this. So, that that exchange is these; so, and there are 3 such mirror planes.

So, there are n/2 mirror plane σ_d which bisect the angles between the $C_2^{'}$ axis and n-2 mirror planes that contain the $C_2^{'}$ axis. So, the 2 prime axis if you are drawing them like this, then there are mirrors containing them as well and mirrors that bisect them also. So, far n odd there are n mirror planes that contain the $C_2^{'}$ axes. So, if n is even then you have both types if n is odd then you get only the containing C_2 axis.

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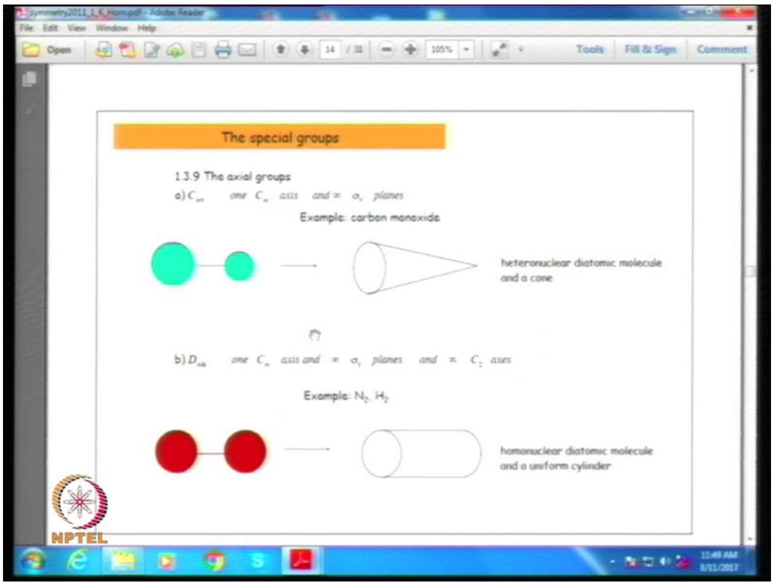

Now come the so, called Special groups, we are not going to use these too much, but just to complete just for completeness and understanding you do have this very highly symmetrical things where you have a just up 2 atom by atomic molecule. So, if the atoms are unequal then you firstly, have a C_∞ axis because you can of course, rotate by any finite any infinitesimal angle as well.

So, about this z axis there is a continuous set of rotations possible. So, it is called C_∞ axis and then there are infinite number of C_v planes because you can draw all kinds of planes that contain the 2 molecules enroute.

So, there is infinity of planes containing the z axis and that is in a sense the symmetry group of the cone, heater on nuclear diatomic molecules and the other example being a cone you. In fact, have a higher symmetry d σ_h; so, D because now there is a plane cutting this axis around which you can mirror reflect and you will remain you have the same thing that is the homo nuclear diatomic molecule.

It has all the symmetries that are symmetry of a cylinder C_∞ axis and infinite number of C_v planes as well as a horizontal axis.

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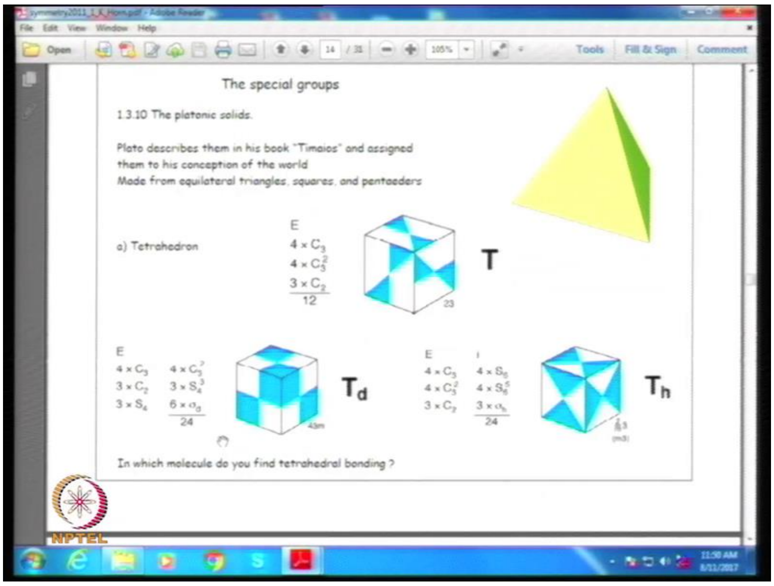

Then come the special groups. So, the special groups and they are not directly useful because nothing in nature comes that highly symmetric, but of course, ammonia has all is almost close to being this ammonia is this it has this symmetry T; it has 24 elements and then the cube group of the cube and the group of the other platonic solids.

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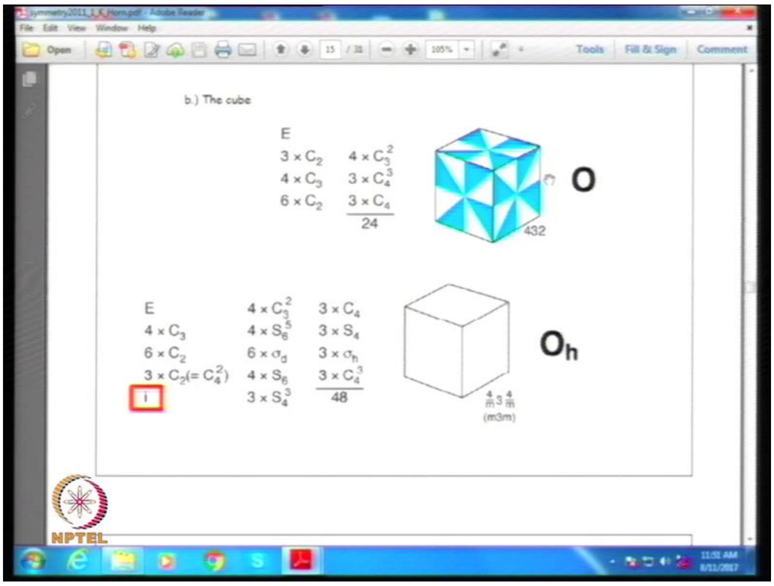

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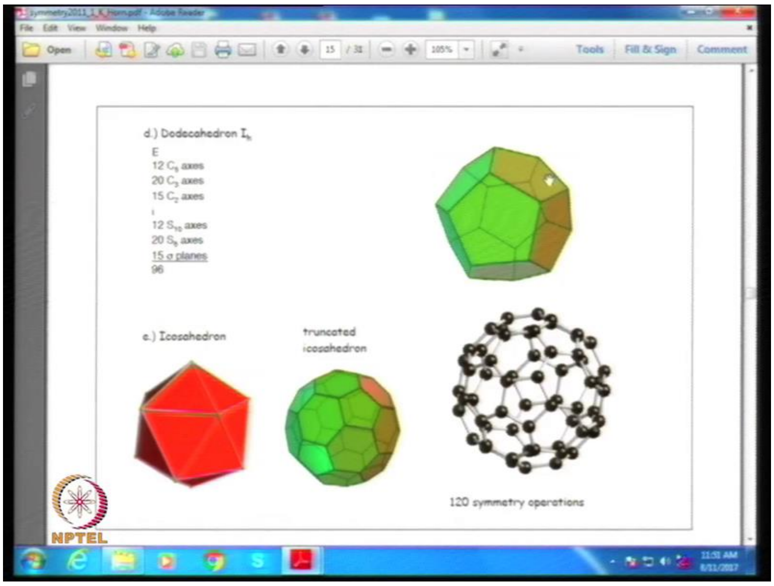

There are totally only 5 as you know the only 5 possible regular polyhedron and there are groups of those.

This C_{60} the carbon molecule became very important fullerene. So, the symmetric groups would be useful there.

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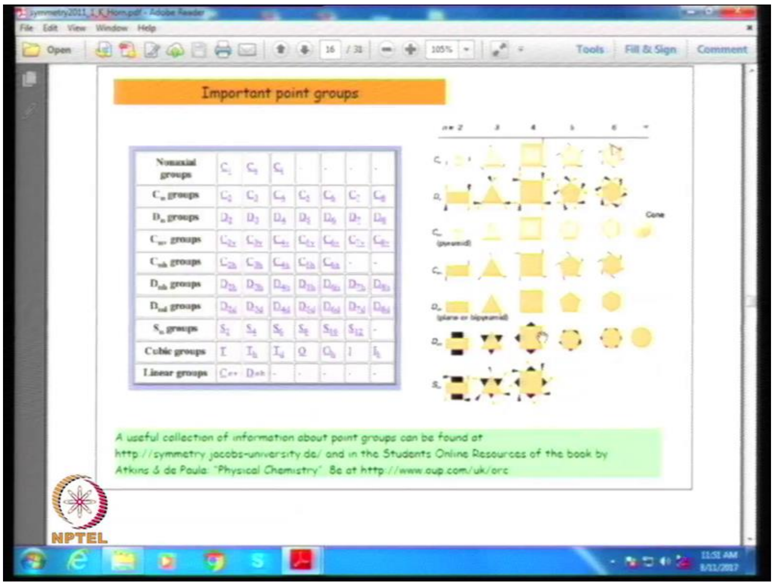

And finally, we end this part of the talk by having the comprehensive list.

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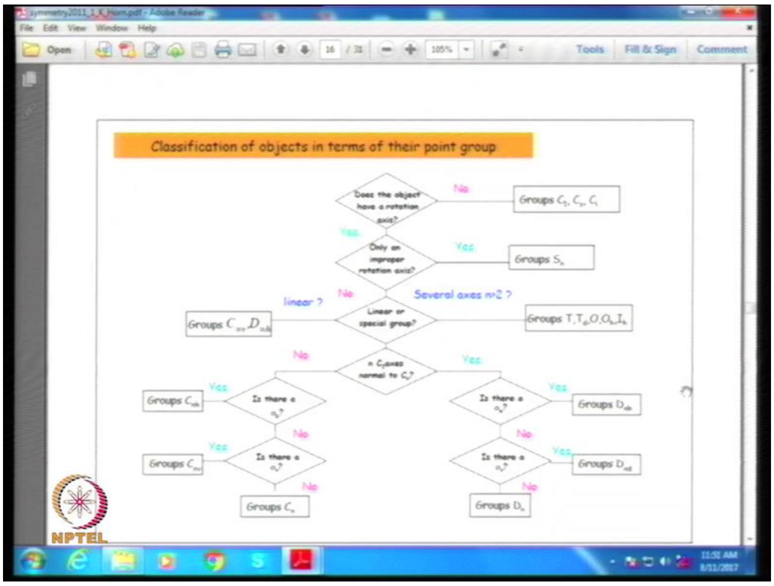

So, 16 is the key slide to look at it has 2 PPT slides in it. One which has a complete list of all the groups that we discussed the non axial group C_n, C_s, C_I and the C_n groups which are just rotations D_n groups that have perpendicular planes C and v that have planes containing the rotation axis C_{nh} which have horizontal axis of symmetry and dihedral symmetry probably C and h is. So, you can look at this table and this is all there is to know about molecular groups and the S_n groups which required necessarily a mirror reflection.

The cubic groups which mostly take care of all the they have not listed probably the higher groups because they probably are composite of the previous groups. And then the linear groups that we just showed that are occur for diatomic molecules. So, this is basically it and, it is worth looking at this and does he points out Jacobs University de also contains all the group theory information. So, two websites I will really recommend is this Jacobs.

Because it has all the character tables which will be using later or you may want to use ever. And the other is this or turbine which has nice simulations or Otterbein is in the US I think near Ohio State University and this Jacobs is in Germany.