Solid State Chemistry
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Lecture – 27
Notation for the 32 Crystal Classes

Now, we will start the second lecture of week 6 of this course. In this lecture, I will be talking about the Notations ok. So, the notations for the various crystal classes ok. So, in the last lecture you learnt all the crystal classes. Now, I will talk about the notations that are used and I will briefly mention the Schonflies notation which is more common for molecular point groups.

But, I will focus on the Hermann Mauguin notation or the international symbols. So, week 6 lecture 2 it will be notation for the 32 crystal classes. And, I will be focusing only on the crystal classes, we will go to the space groups little in the next lecture, that will focus on in this lecture on the crystal classes ok.

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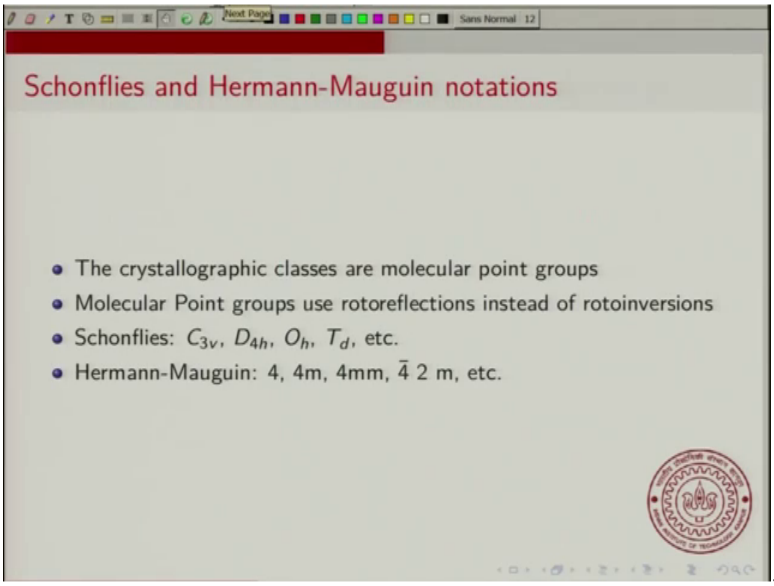

So, there are two common notations that are used; one is called the Schonflies notation and the other is a Hermann Mauguin notation. And, you should keep in mind that the crystallographic classes are essentially similar to molecular point groups.

These are like molecular point groups for objects for the outer shape of the crystal. And, conventionally molecular point groups use rotor reflections instead of roto inversion. So, in crystals we used to use roto inversions whereas, in molecular point groups roto reflections are used. Now, the Schonflies notation you might have seen in molecular group theory ok. So, there are terms like C 3v, D 4h, O h for octahedral td for tetrahedral and so on.

The Hermann Mauguin notation this is something you might not be so, familiar with, but in this the names of the point groups are just like numbers like for 4 m, 4 mm, or 4 bar 2 m, etcetera. So, typically up to 3 3 numbers and we will see what kind of combinations are there.

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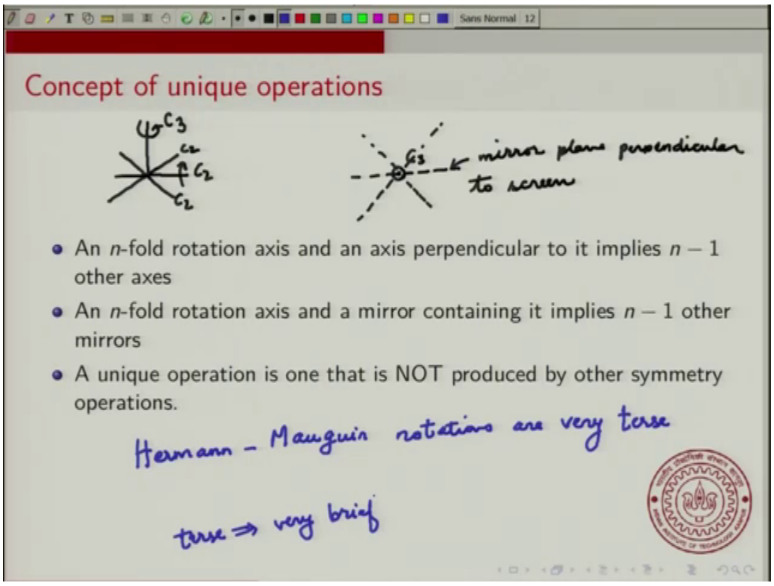

So, now in order to understand the Hermann Mauguin notation and in particular the Hermann Mauguin notation, we need a concept called unique operations ok. The idea is that if you look at the total number of symmetry operations; so, I will just step back a little bit.

So, for example, the octahedral point group ok. Now, you know that it has a very large number of operations; it has 48 operations ok. And, that indicates of the presence of all these 48 operations. Now, it turns out that not all these 48 are unique ok, some of them are not unique ok, some of them are implied by the existence of others.

So, so, the concept of a unique operation is can be understood in the following way. So, suppose you have an n-fold rotation axis and an axis perpendicular to it another rotation axis that is perpendicular to it ok.

So, so, you could have something like this you have a you have a let us say there is a C 3, if you have a C 3 axis. And, let us say you have in the plane perpendicular to it you have a let us say a C 2. So, the C 2 is perpendicular to the C 3 ok.

Now, this automatically implies. So, having a C 3 automatically implies that you should have 2 more C 2s ok. So, there will be 2 more C 2 axis which are basically 120 degrees from rather it will be you will have 2 more C 2 axis that will be oriented like this and like this.

So, these are again these are perpendicular to the plane of the paper ok. So, basically this implies 2 more C 2 axis. So, , in a sense one of these C 2 axis is unique the other two are implied by the presence of this perpendicular C 3. So, this gives you an idea of where the concept of unique axis comes. Similarly, if you had a if you had a let me let me look at this screen if you have if you had a mirror plane, and you had a C 3 axis let us say perpendicular to this mirror.

So,. this is a C 3 that is perpendicular to this that that contains the mirror and it is perpendicular to the screen. So, this is a mirror mirror plane I am showing it by dashed , but it is perpendicular to the screen of the paper, perpendicular to the screen. And, now if you have a C 3 axis; so so the C 3 axis is actually coming out of the screen of the paper. So, this C 3 axis is actually coming out of the screen ok and, now so, so the C 3 axis is perpendicular and it contains this mirror.

So, the so, this is the mirror the C 3 axis lies in the mirror ok. And, what this implies is that it automatically implies that there should be 2 more C 3 axis or 2 more mirrors, it indicates that there should be 2 more mirrors and I will show them, there will be one this way and one in this direction. So, it automatically indicates that there should be 2 more mirrors. So, the point is that one of these mirrors is unique the other 2 are implied ok, by the by the existence of C 3 and the first mirror.

In other words a unique operation is an operation that is not produced by other symmetry operations. So, so you can think of one of these mirrors as produced by this mirror followed by a C 3, a combination of C 3 operator on one mirror will give you another mirror. So, a unique operation is one that is not produced by other operations ok.

So, so this is a way to this concept of unique operations will be essential in describing the symmetries, or in identifying the Hermann Mauguin notations. Now, one of the one of the very important features of this Hermann Mauguin notation ok, and I will emphasize this ok.

So,. Hermann Mauguin notations are very very terse ok. I am using the word terse terse basically means they are very brief. So, terse means very brief ok. So, they are very compact notations ok, they are very compact notations. And, essentially through these very compact notations, you are you are you are showing the entire set of symmetry operations of a point group ok.

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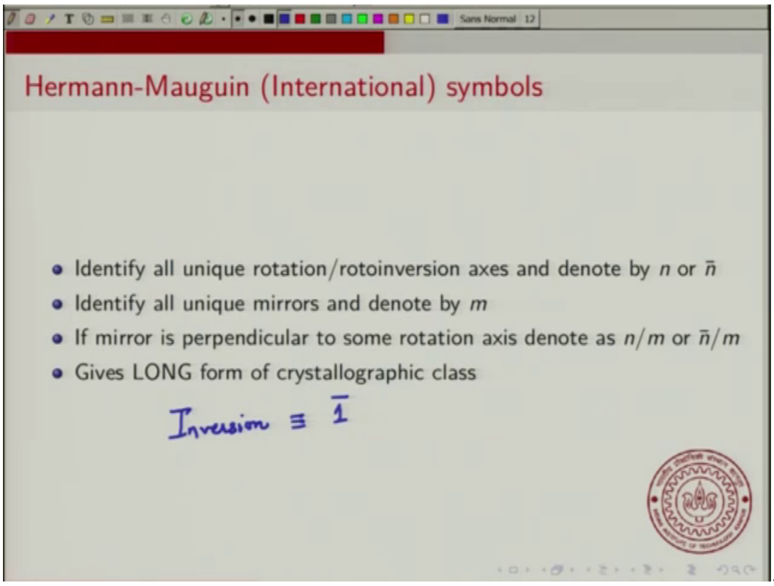

Now, the so, so coming to the Hermann Mauguin international symbols ok. So, this is a procedure for identifying the Hermann Mauguin international symbols. So, what you do is first you identify all the unique all the unique rotation or roto inversion axis and denote them either by n or n bar.

So, identify all the unique roto inversion axis and denote each of them by the letter n or n bar ok. If, it is a roto inversion you will use n bar if it is a for example, if you have a threefold roto inversion you will use 3 bar ok. If you have a 4 fold rotation you will just use 4 ok. So, you so, you identify all ok. The, important word is all the unique rotation or roto inversion axis and denote them by n or n bar, and you can show that you cannot have more than 3 of such unique rotation and roto inversion axis.

So, you can get maximum 3 3 of these numbers. Next, what you do is you identify all unique mirrors and denote them by m ok. So, you see how many mirrors these are mirror reflections. So, how many how many mirror reflections mirror planes are there, identify all of them and look at which ones are unique and you denote them by this letter m.

So, these are the first 2 steps and again you can show you cannot have more than 3 unique mirrors ok, in a in a 3 dimensional crystal. Now, if a mirror is perpendicular to some rotation axis, then you denote it as n by m.

So, if m is a mirror that is perpendicular to a rotation axis n, then you denote the axis and you put a slash between the axis and the mirror symbol. So, you denote it as n n by m. Similarly, if it is perpendicular to a roto inversion axis n bar then you denote it as n bar by m ok. And, just these 3 operations it gives the long form of the crystallographic class. And, in this lecture I will focus on the long form of the Hermann Mauguin international symbols ok, that gives you the crystallographic class.

So, that is all you need to do and as we said crystallographic class only refers to rotation and reflection. Now, you might ask what about what about the inversion center. Now, the inversion center is nothing, but 1 bar ok. So, so we keep in mind that inversion is equivalent to 1 bar. So, it is included in 1 bar ok. And, , so this essentially you can you are taking care of all the symmetry elements of this crystal ok, of all the of the point group of the crystal ok.

So, now, let us look at some examples ok.

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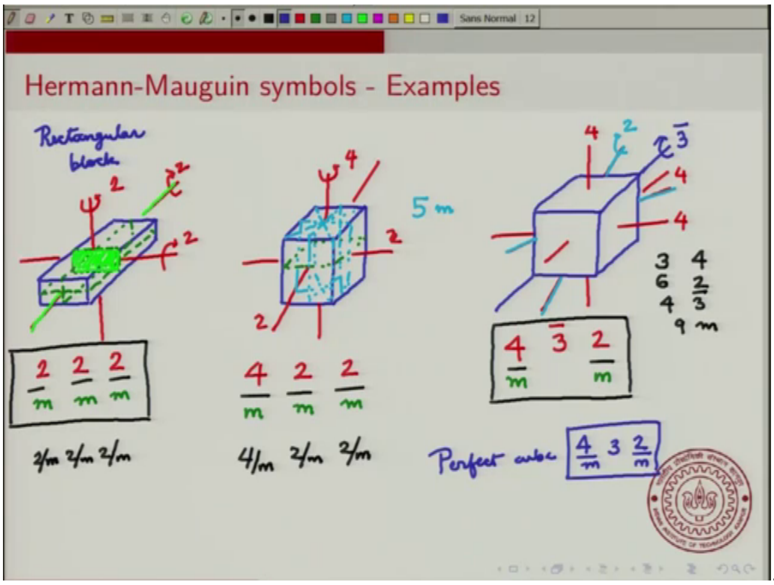

We will take some very simple examples that will that will tell you how to how to do this? So, first let me take a rectangular block and I will just show it like this. So, you have something like this perfect rectangular block ok. So, now, now let us let us write the Hermann Mauguin symbol for the point group of this of this block. So, the first step is to identify all the symmetry axis. Now this rectangular block has all sides different ok.

So, the only rotations that are there are essentially there is a there is a 2 fold axes of rotation this way. So, 2 fold axes of rotation, then there is a 2 fold axes of rotation that goes this way, and another 2 fold axes of rotation that goes in this direction. So, there are 3 2 fold axes of rotation; so, we will write 2 2 2. Now are there any other rotation axis in this rectangular block no there is no other rotation axis in this rectangular block, what about the mirrors, what about the mirror planes?

Now, again you can see that I will just you can see I will just show it by a dotted line that intersects. So, if we imagine that there is a mirror that goes this way this would be a mirror plane ok.

So, it contains it contains this it contains this axis and this axis. So, it is a plane containing this axis and this axis ok. So, you have a mirror. And, similarly you can have 2 more mirrors ok, there was that contained one and one that look like this ok. And, a third one that will contain that will be perpendicular to this ok.

So, those would be the 3 mirror axes. So, 3 mirror planes. So, you have 3 mirror planes. And, notice that each of these mirrors is perpendicular to one of the axis.

So, for example, if you take let me shade it in light green. So, if you take this mirror, that is perpendicular to this axis ok. So, this mirror is perpendicular to this so, C 2 axis. And, similarly the other 2 mirrors are also perpendicular to the axis. So, we can just put dash between this, you can write it as 2 by m or if you are writing in a single sentence you can just write it as 2 slash m ok.

So, so the so, this is really the point group. So, the point group of this rectangular block is 2 by m 2 by m 2 by m ok, you can you can write it as if you are writing in a single sentence, you can write it as 2 by m 2 by m 2 by m ok. This is the point group of this rectangular block ok.

Next, let us consider something that is slightly different ok. Let us take a take something that is again it is rectangular, but it is, but there are one of the sides is a square. So, , if you have if you have something like this and this side is a square ok. Now, what you have is you have now this axis of rotation becomes a 4 4 fold axes ok. And, the other 2 2 fold axes remain as they are. So, these 2 continue to be 2 fold axes ok. So, these 2 continue to be 2 fold axes , but you have a 4 fold axes. So, this is a 2 fold axes, this is a 2 fold axes. Now, what about the mirrors? Ok.

So, we can we definitely have 1 mirror that is perpendicular to this 4 fold axes. So, so we have one mirror that is perpendicular to this 4 fold axes and I will show it in this way ok; so, let me write. So, you have a 4 you have a 2 and you have a 2 ok. And, we definitely have a mirror that is perpendicular to this 4 fold axes. So, so then I will have a 4 let me put the slash and an m. Now, again now you have you actually have the mirrors containing this I will show them I will show them here ok.

These are so, you have a mirror that is perpendicular to the 2 axes 2 to this 2 axes. So, you have this mirror ok, you have another mirror that contains the other ok, that is perpendicular to this 2 axes to. So, , this mirror is perpendicular to this 2 axes and this mirror is perpendicular to this 2 axes , but there are 2 other mirrors there are 2 other mirrors. And, I will just show the one will be this way and one will be in this direction and I am going to show the full mirror ok.

So, actually you have a total of you have 4 plus 1 5 mirrors 5 mirrors ok, but you can easily see that you have a mirror perpendicular to this 2 and a mirror perpendicular 2, this 2 ok. And, because of this 4 fold symmetry ok, this 1 mirror it automatically implies 3 additional mirrors ok. So, what I mean to say is that not all of these are unique and we just write the mirrors that are perpendicular to these ok.

So, out of these 5 mirrors ok, we write only 3 of them. And, in fact, actually truly only 2 of them are unique, but since the since you also have one that is perpendicular to this 2 we write that also. So, the space group now is 4 by m, 2 by m, 2 by m ok.

Now, the third example I am going to do is that of a cube ok, slightly we will just make it a little more complicated than a regular cube ok. So, we imagine that you have a cube, but now we assume that this C 3 you do not have C 3 axes, but you have 3 bar axes this is a 3 bar axes.

So, you have 4 instead of having 4 3 axes threefold axes you have 4 3 bar axes. So, this is not a this not a perfect cube you imagine that there is something that that is that makes this that converts this 3 axes into a 3 bar axes. So, we have 4 3 axes 4 3 bar axes and now and now you can write.

So, you still have the 4 fold axes ok. So, the 4 fold axes is still there as it is. So, you have this and so, you have so, you have so, you have 3 4 fold axes. So, this is a 4 4 and a 4. Now, notice that out of out of these there is only there is only one unique axis here ok. So, because you have a 4 fold axes ok.

If, you have one axis of rotation then this is the second one is automatically implied. So, so, if you take this 4 axes and this 4 axes then it automatically implies this for a actually it imply it implies 2 other 4 fold axes which are which we are not showing here to you it also implies 2 other 4 fold axes ok. But, there are additional axis that are there and that is this 2 fold axes. So, for example, you have 1 2 fold axes like this ok, coming from you know you know going through the center of one face and coming out on the other side ok. So, you have these 2 fold axes.

And, again you can you have you have a total of 6 of these 2 fold axes ok, but again their only one of them is unique because of all these 4 fold axes. So, you have a 4, you have a 3 bar, and you have a 2 ok. So, this is a 2 fold axes. So, this let me use a slightly different color just for the 2 fold axes. So, this is a 2 fold axes this is another 2 fold axes and there are a total of 12 of them 2 fold axes.

So, actually the you have if you if you look at the total number of operations you have 3 4 fold axes, you have 6 2 fold axes, and you have 4 3 bar axes.

However, the you can you can easily show that only one of these 3 bars is unique and only one of these 2 2s is unique ok. And, now if you take the total number of mirrors you have a total of 9 mirrors ok. And, again this is not very hard to show you have 9 mirrors ok. And, the mirrors are actually perpendicular to the 4 axes and the 2 axes there is no mirror perpendicular to the 3 axes the 3 bar roto inversion axis ok. So, you can put slashes here put the mirrors and this is the space group symbol.

So, now, you have the space group symbol for this cube that has a 3 bar instead of a instead of a you know instead of a perfect 3 3 fold rotation, this is you know slightly you can think of this as some sort of unsymmetrical cube ok. Now, if you had a if you had a perfect cube if you had a perfect cube ok. Then you can easily see that will be 4 by m, 3 3 3 2 by m. So, so the long form for the perfect cube will be 4 by m 3 2 by m ok. So, now, with this with these examples we will just list all the notations for all the crystal classes and, we again we will start with the most unsymmetrical.

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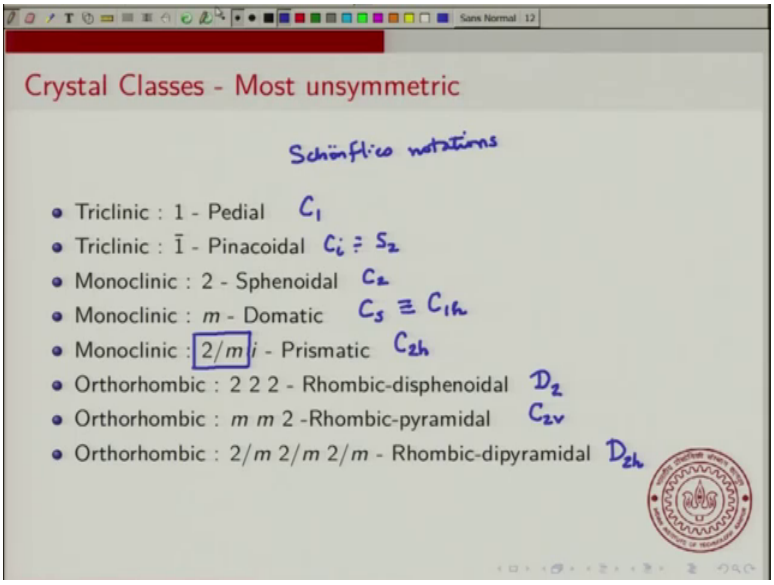

So, the most unsymmetrical is the triclinic system ok, it is called the PDL class and there is just a 1 ok.

So, so, the only there is one is just the identity there is no symmetry operation. So, the so, the class notation is just 1 ok. So, so this is the Hermann Mauguin symbol ok, the Schonflies symbol for this is C 1. The second is the Pinacoidal where it is 1 bar is the only symmetry. So, it has a center of inversion ok. So, you just denoted by 1 bar, in the Schonflies notation you either use C i or you use S 2 C is equivalent to S 2.

Similarly, the sphenoidal has only 2 2 fold axes. So, this would be a C 2 group in the Schoenflies. So, these are the Schonflies symbols Schonflies. Similarly, the monocline the if you just have a mirror then the Hermann Mauguin symbol is just m for the space group here the here this is actually denoted as C s or C 1 h ok.

So, h reflects the fact that you have a mirror plane ok, now what about 2 by m 2 by m 2 by m now the Hermann Mauguin notation ok. So, we said that 2 by m automatically implies an inversion center. The Hermann Mauguin notation is just 2 by m ok.

And, again the inversion center is not necessary, because for the Hermann Mauguin notation. The in the Schonflies symbol you would write this as C 2 h ok. Now, what about the orthorhombic group so, the 2 2 2 ok. So, you can have a Hermann Mauguin notation 2 2 2 the Schonflies symbol is D 2 ok. And, the mm 2 would be a C 2 v I will just note this and then this is D 2 h.

Again so, the so, you see that that the existence of the mirror, you these are the symbol 2 is used C 2 or D 2 implies a 2 fold axes of rotation. And, then and there are various symbols to indicate the directions of the mirrors of the mirror planes ok. Now, again we would not be talking too much about the Schonflies notation, but it is, but you know it is likely that you will see it in some cases.

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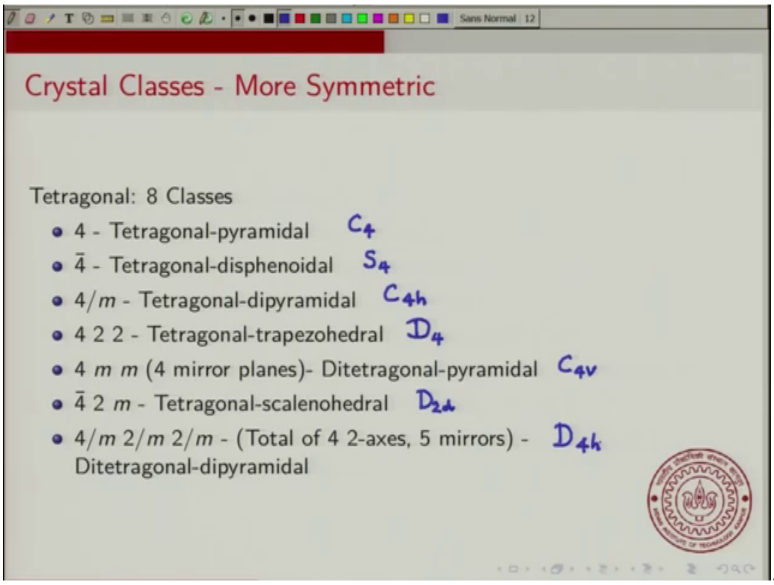

Now, let us go to the groups to the tetragonal groups ok. Now, if you just have a 4 fold axes then the Schonflies notation is C 4, if you have a 4 bar then the Schonflies notation is S 4, then you have a 4 by m then it is C 4 h if you have a 4 2 2 ok.

Now, the Schonflies symbol is just d 4 ok. Similarly, if you have 4 mm this is C 4 v ok, the 4 bar 2 m this is D 2 d and then the 4 by m 2 by m 2 by m, this is denoted as D 4 h ok. So, these are the tetragonal groups.

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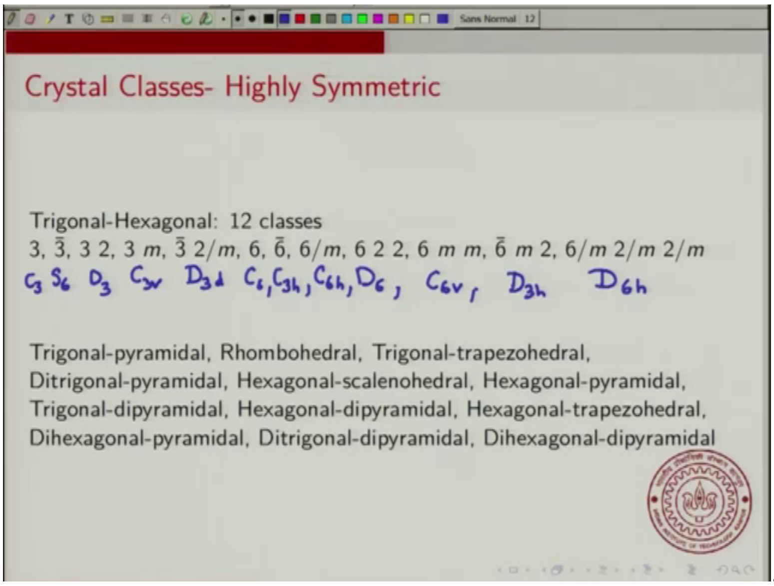

Now, I would not list all the trigonal hexagonal ok. I will just say that this is C 3, this is this is actually C 3 and I this is an s 6 ok. And, then this you have D 3 you have D 3 d, this is 3 m corresponds to C 3 v this is D 3 d, 6 is just C 6 s this 6 bar is actually denoted as C 3 h. And, 6 by m is denoted as C 6 h ok. This is 6 2 2 is denoted as D 6 ok. Again, I do not expect you to know all these; however, however you can tell by looking at the symbol that that you have a threefold axes or a 6 fold axes.

And, so, , let me just list the last one this one it is called D 6 h ok, and I mean we can just complete the set. So, the 6 bar m 2 is denoted as D 3 h and 6 bar mm is denoted as C 6 v ok; so these are the Schonflies notation. Now, I mean if you are familiar with molecular group theory you will recognize that v stands for a vertical mirror, h stands for horizontal mirror, and d stands for diagonal mirrors , but again I am not going to emphasize all these names ok. So, so, I would not expect you to know all the Schonflies symbols, nor would I expect you to know all the names of these crystal classes.

So, other than the most symmetric or the least symmetric I would not expect you to remember all these names.

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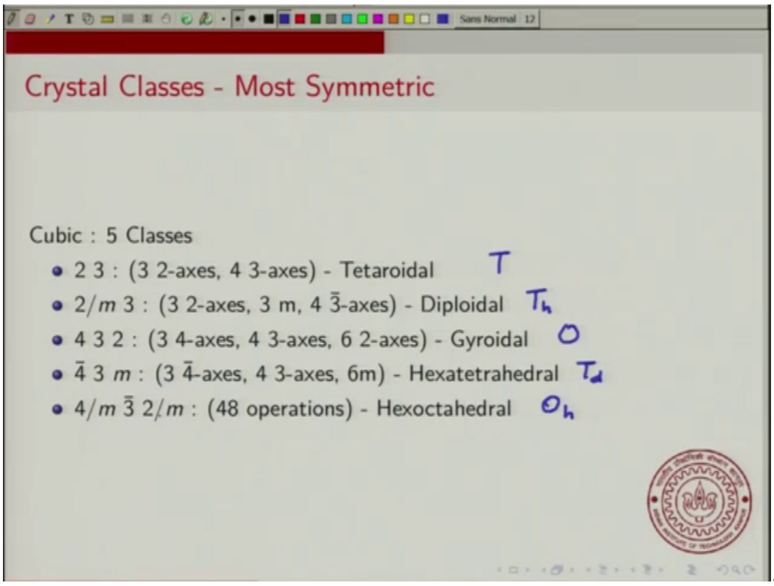

And, let us complete it. So, the cubic class is 2 3 ok, 2 3 is there is a Hermann Mauguin notation in this is tataroidal the symbol is just a t ok. So, and then this is T h, this is O, T d and this is O h ok. So, the 48 operations the group which is 4 by m 3 bar 2 by m 2 by m this is the octahedral point group.

So, you can look at all these point group symbols ok. And in some sense there is a logic in all of them ok, definitely the Hermann Mauguin notations can be derived for the most part.

There are some conventions that are used, but for the most part you can derive them. The Schonflies symbols yes there is some there are some conventions there also and you can you can understand these conventions based on the symmetry operations in the point group. So, next we will extend this discussion ok, we will talk about a more truncated form of this Hermann Mauguin notations called the short form and then we will extend the discussion to space groups.

Thank you.