Solid State Chemistry
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Lecture –29
Hermann – Mauguin notations for Space Groups

Now, I will start the fourth lecture of week 6 of this course. In this lecture, we will look at the Hermann-Mauguin notation for the Space Groups and this very will actually conclude our discussion on the on the notations and also conclude our discussion on symmetries. So, week 6 lecture 4 Hermann-Mauguin notation for Space Group.

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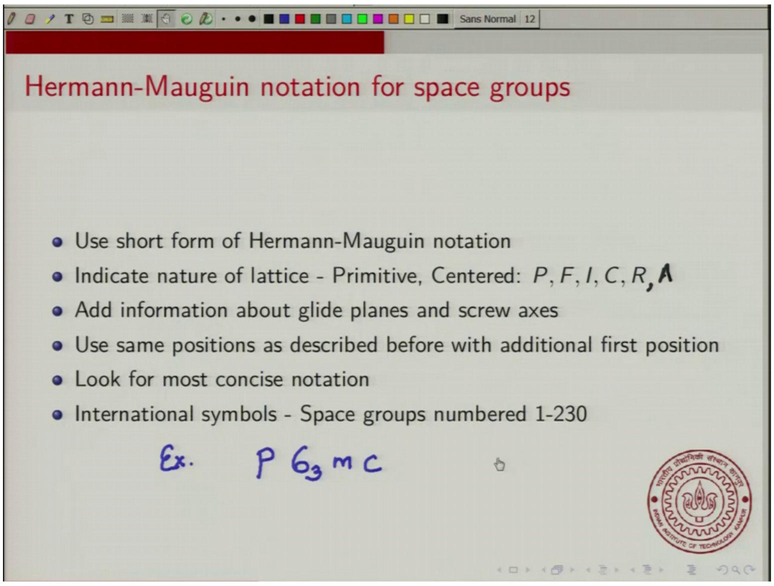

So, some general rules in writing the Hermann-Mauguin notation, you can use the short form of the Hermann-Mauguin notation. There are also cases where the long form is used, but we will stick to the short form and we will indicate the nature of the lattice ok; that can be primitive or centered it can be P F I C R. There is also a possibility of having an A center that we will see in some special cases. R is only for the R centered a hexagonal lattice. Then, so, so use a short form and indicate the nature of the lattice. Then you add the information about glide planes and screw axes and when you do this, so we so will actually look at each position; the first, second and third positions of the Hermann-Mauguin symbol and we will see whether there is a whether there are glide will glide planes or screw axes on these positions. And then, and then again we will use the we will use the same position with an additional extra position that is the that indicates this symmetry ok.

So, I will just give one example ok. So, you can have something like P 6 3 m c ok. So, you can see that the first position is this is an example ok. So, we can see that here the P indicates primitive ok; the 6 3 indicates that there is a 6 3 screw axis at the first position and then a mirror at the second and a c glide at the third position and again, as always we will use the most concise notation, we look you have to look for the most concise notation and these are also called international symbols.

And you can also in the space groups are also numbered 1 to 230. So, the space groups you have 230 space groups for all crystals and these are numbered 1 to 230 and so, I won't be discussing all the 230 groups ok. But I will try to give you a feel for some of these numbers ok. So, that so that when you see them in while reading other books or learn or reading about different crystals, then you are not completely unaware ok.

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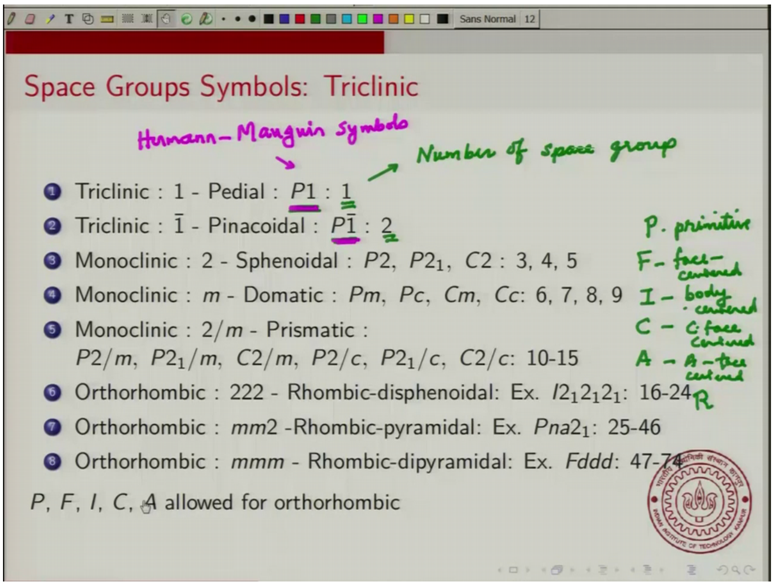

Let us now look at the space group symbols. Now in the case of the triclinic system ok; there is only 1 space group possible ok. There in the orin the in the case of the pedial system, there is only 1 space group and that is just denoted as 1 the pinacoidal is just a 1 with an inversion ok. And this last digit here is actually the number ok. So, this is the number of space group ok. Some crystal that is that is whose space group is numbered 1, then it corresponds to the triclinic period the nomenclature is P 1. So, this is the

Hermann-Mauguin symbol. This is the space group number. So, so P 1 and P 1 bar or Hermann-Mauguin symbols ok. Let me use a different color to indicate that. So, these are the Hermann-Mauguin symbols; Mauguin symbols ok. So, then the then you go to then you go to the others like in the case of Monoclinic the sphenoid case, now in the Sphenoid crystal class there are actually 3 different space groups that are possible ok.

You can have a P 2 primitive two that only has the 2 twofold axes. Now you can have a P 2 1, where the twofold axes is actually a screw a screw axes of rotation. Then, you could have a C 2 ok. C is a C centered and you donot have a primitive, but you have a C centre 2 and these are numbered 3, 4, 5. Then you can have the Monoclinic Domatic ok, where you have to have a mirror. Now you that so you could have in the in you could have primitive with a mirror, primitive with a c glide plane or a C center with a mirror C center with a glide plane and these are denoted these are given the number 6, 7, 8, 9. Now, if you have the 2 by m the prismatic crystal class; now you have you have a total of 6 space groups. You can have a P 2 by m just a primitive 2 by m P 2 under script 1 that is a screw axes in the perpendicular mirror. Then have a C center and a 2 by m P center and a 2 where the mirror is actually a C glide; P center and screw axes and the mirror is a C glide; a C center with the 2 axes and a C glide right ok. Now, notice that not all the combinations are there ok, there are certain restrictions ok, there are certain restrictions on which is allowed for which one for example, you donot have a C center with whether 2 axes is a 2 is a is a screw is a screw axes ok.

And that that is indeed the case and you know these are not you cannot have arbitrary symmetry operations. These have to satisfy the lattice condition. You can now the orthorhombic we have the 2 cross 2 Rhombic-disphenoidal class ok. So, one I will just give one example actually there are there are a total of 9 different space groups ok; space group number 16 to 24 fall in this ok. I will just give one example. This is the this is a I means it has a body centered. So, I will just make a few points here. So, so P means primitive; F means face centered . So, this is for the first alphabet of the of the space group.I is body centeredand addition C is C C-face centered and then, A similarly A also A-face centeredand you can also have will also see that you can have an R which is an R-centered ok.

So, these are the possible numbers that you can have. In this case I means a body centered 2 1. So, the 2 axes that you have that you are supposed to have for to be orthorhombic though each of them is a is a 2 1 screw axes ok. Now the Rhombic-pyramidal class that is mm 2 ok; now an example of this is P n a 2 1 ok. So, what this means is that the first position mirror is actually an diagonal glide ok. So, that that mirror is a diagonal glide reflection symmetry. The second mirror is an a glide and the 2 the twofold axes of rotation is a screw axes 2 1 screw axes and this Orthorhombic mm 2, this is just one example ok, but in this Rhombic-dipyramidal crystal class, there are actually there are there are 22 different space groups in this..

So,from numbers 25 to 46 are in this space group. Then you can have the Rhombic-dipyramidal, where you have the mmm an example of this is a face centered ddd, where each of the mirrors is a diamond glide and this is one example ok. There are you know there are several different space groups in this and the total number of space groups here takes it from goes all the way from 47 to 74. So, there are a total of 28 space groups in the Rhombic-dipyramidal crystal class and from the Orthorhombic system, you can have primitive; you can have face centered; you can have body centered; you can have C center or A center. Now again, again the C and A ok, these have to be looked at with respect to the position. So, the first position is usually reserved for the C; C axes and so, so you it turns out you can have both C and A center ok.

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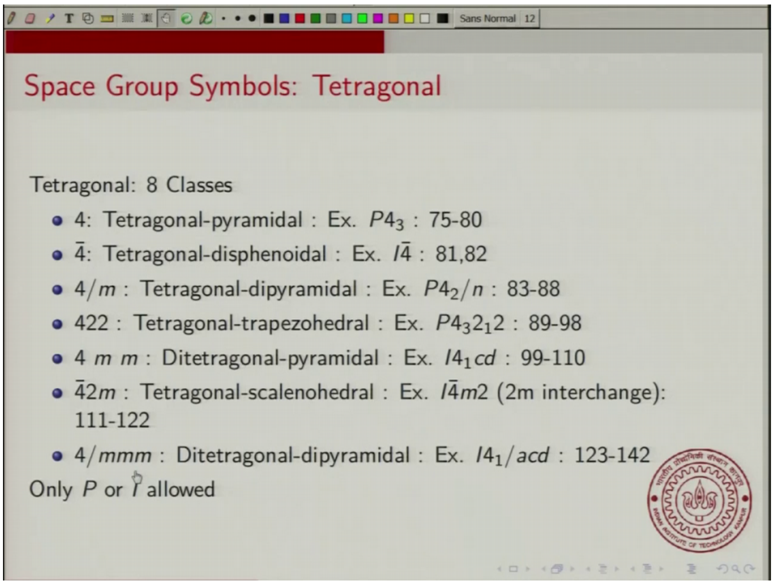

What about the Tetragonal? Now the Tetragonal-dipyramidal, where the crystal class is just denoted by 4 in this case you can have a total of 6 space groups. So, they range from numbers 75 to 80; one example is P 4 3. So, its primitive and the fourfold axes is actually a 4 3 screw axes ok. Then you can have 4 bar here there are only two different space groups 81 and 82. So, one example is I 4 bar.

So, you can just have the 4 bar without anything and you can have the 4 bar with a bob with a inversion center. The 4 by m that is a Tetragonal-dipyramidal, in this case there are there are a total of 6 space groups ok. One example is a P 4 2 by n. So, the. So, here the fourfold axes is actually a 4 to screw axes; the mirror is a diagonal glide ok. Then there are if you take the 4 two 2 this is a Tetragonal-trapezohedral crystal class and now there are 10 space groups in this in this crystal class. Here is an example where you have a 4 on subscript 3 2 subscript 1 and 2. Then you can have a 4 mm which is a Ditetragonal-pyramidal, in this case you have you have I. you have a total of 12 12 space groups; they go from 99 to 110. One example is a I 4 subscript 1 cd.

So, the first position the fourfold axes here is 4 1 screw axes and the second mirror is a c glide and the third mirror is ais a is a diamond glide ok. So, and this is this has a center of inversion. So, so it is so the first letter is I. Then, theTetragonal-scalenohedral ok; now here again you have you have 12 12 different space groups and this is characterized by 4 bar 2 m. An example is shown here, notice that this particular example the where I had a 2 I have an m and where I have an m I have a 2 ok. This is very special ok, it does not happen too often ok. So, the twofold axes is actually replaced by a mirror and the mirror is replaced by a twofold axes. So, so there is some I mean this is extremely special; I mean you very rarely find this in interchange between 2 and m ok.

But in this case it does happen and again, again that has to do with this with this with this location. So, you have a m and a 2 m the second position and the third position they are They arethe idea is to have a consistent notation so that you can from this name you can work out what are the symmetries of the crystal ok. So, therefore, the second position and the third position are perfectly defined ok. The first second and third positions all thesepositions are well defined. Now this is another class ok. So, you have a 4 by mmm ah. So, this is a Ditetragonal-dipyramidal ok; an example is I 4 1 by acd ok. So, the first mirror that is perpendicular to the fourfold axes is now an a glide and then the second and third mirrors are a c glide and a diagonal glide and this has fairly large number ofnearly 20 20 space groups in this. So, so the tetragonal class is involves you know it goes all the way from 75 to 142 ok. So, there are quite a large number of space groups that are in the tetragonal class., in the tetragonal class only primitive or body centered are allowed. So, it can only be either primitive or body centered; you cannot have a face centered tetragonal or a c centered tetragonal.

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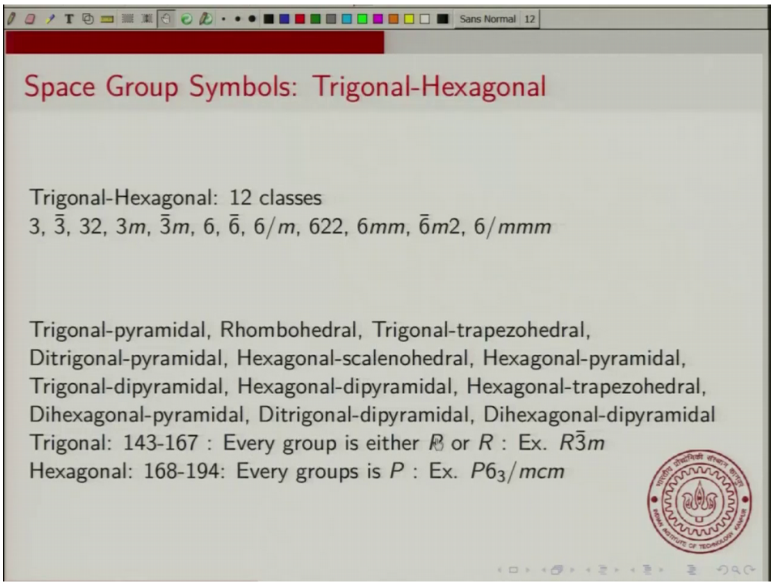

Next we will go to the trigonal hexagonal and here, here we have the 12 classes; the 12 space groups. These are the 12 12 point groups. These are the short forms ok. I will just give a few examples ok. So, the now the Trigonal goes all the way from 143 to 167 and here every group is either primitive or R centered ok. An example is R 3 bar m ok. So, the trigonal basically goes in this set ok. The hexagonal in this case every group is every group has to be primitive ok. An example is P 6 3 by m c m ok. so, that would fall in this in thisin this crystal class and that crystal class is Dihexagonal-dipyramidal ok. So, this goes for all the way from 168 to 194ok. So, so the trigonal hexagonal and the in the tetragonal crystal systems ok, they have a fairly large number of space groups.

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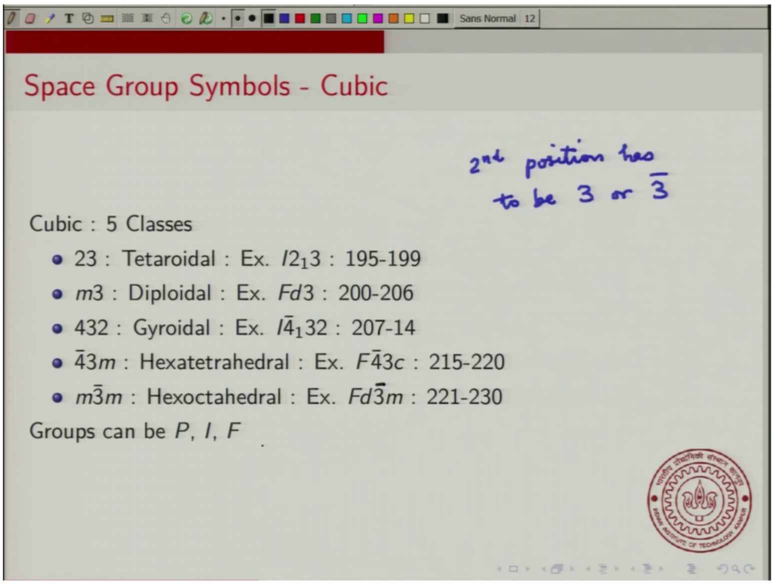

Finally, we go to the Cubic crystal class ok. Now here the here you have the 5 you have the 5 different classes ok. There is a there is a tetaroidal and this the space groups for tetaroidal go from 195 to 199. So, there are only 5 of them the Diploidal has goes from 200 to 206. In the tetaroidal notice you have a 2 and a 3 ok.

What is important for the cubic crystal system is that is that the second position has to be 3 or 3 bar ok. So, this is a condition for the cubic system. So, the second position has to be either 3 or 3 bar ok. The first position is usually a some sort of higher, I mean it can be a higher order axes; it can be a mirror or it can be even enrolled lower ordered axes ok. So, the tetaroidal and diploidal in that in that the first position is actually a twofold axes and a mirror. These are examples of these 2 classes; examples of space groups in these 2 class classes..

The Gyroidal has 4 3 2 ok. So, one example of a space group in this class is I 4 bar 1 3 2 ok. So, you have a fourfold roto inversion and say it is actually a 4 1 roto inversion screw axesok. Then there is a 3 which is the middle number and then and then you have a 2 at the end. So, you have a 2 fold axes also. And actually this wholeclass of gyroidal goes from 207to214 the hexatetrahedral which is 4 bar 3 m, again there are many space groups; there are a total of 6 space groups for this and they one example is shown here F 4 bar 3 c. So, the mirror is actually replaced by a is a is a glide reflection..

Then, the Hexoctahedral which we saw in the short form as m 3 bar m ok; an example of this is F d 3 m here. So, this goes from 221 to 230.It should be a d 3 bar m ok. So, this goes from 221 to 230. So, there are 10 groups in this ok. So, the cubic system cubic groups can be either P, I or F so, but what is important is that second position has to be 3 or 3 bar ok.

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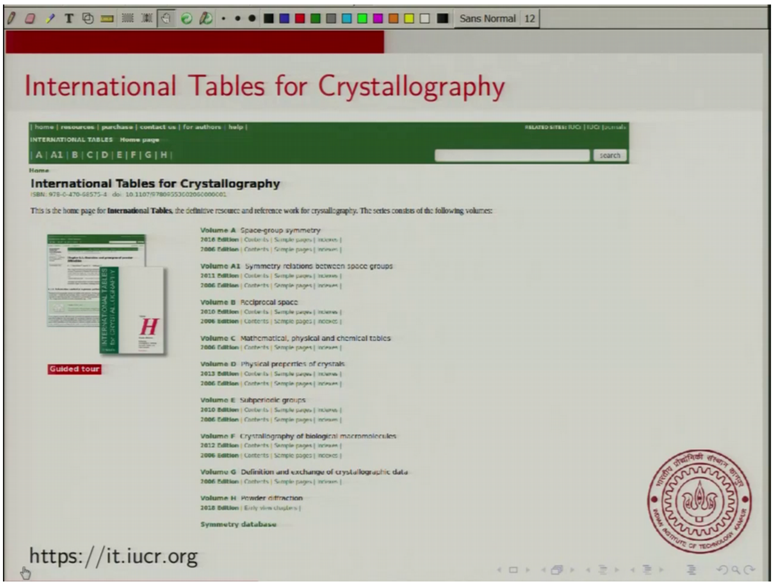

Now, before I conclude this lecture, I want to tell you that you know identifying space groups is not very easy and there is a there is a very nice resource for space groups and lot of properties of crystals ok. This is the international tables of for crystallography ok. This is the website the website for that is shown here ok. So, this is the website for this international table of crystallography. You can actually buy this ok; you cannot it is not a free download. But you can you can buy these international tables for crystallography.

And these are usually available in most colleges and institutional libraries and what is important is that they keep updating some of these. So, as more so in fact, so, there is space group symmetry there is symmetry relations between space groups, there is a reciprocal space which will come and then there is there are other tables and lot of things ok. But the, but the space group symmetry contains all the information about you about all the different space groups ok. In addition to this, there are also some online resources which also which also they give lot of these information about space groups ok.

So, so I will I will conclude this lecture here and I will in this in the next lecture, we will summarize what we learnt in week 6 and do some practice problems, but I want to make a few points ok. See there are 230 space groups. It is not possible that you will remember all of them ok, but I would expect you to have some idea about the different crystal classes andsome idea of what kind of space groups you can have and when we work out some examples, we will we will look at someat least at least for the simple for the crystal classes that do not have too many too many too many space groups ok.

You can you can be expected to at least know some of the different space groups. So, for example, like triclinic monoclinic ok. I would expect you to know some of the some of the space groups ok. Additionally, we said that we said that there are some very special things about the names like for example, in a cubic you can have either P, I or F and similarly in a cubic the second number has to be a 3 or a 3 bar ok. So, these are some of the little things that will help you to quickly identify space groups ok.

So, you know you know just by looking at the name of the space group, you can you can usually tell at least at least you can tell broadly which crystal system it belongs to. Beyond that in some cases you can tell the crystal class and in some cases you can actually identify the detailed of the space group ok, just by inspecting the name. Of course, I am not saying it is very easy. So, we will look at some simple examples and at least at least for simple cases, I would expect you to be able to work out these things ok. So, I will conclude this lecture here. In the next lecture, we will review what we learnt in week 6 and do practice problems.

Thank you.