Crystal, Symmetry and Tensors
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3D Space Groups Vll:
73 Symmorphic Space Group

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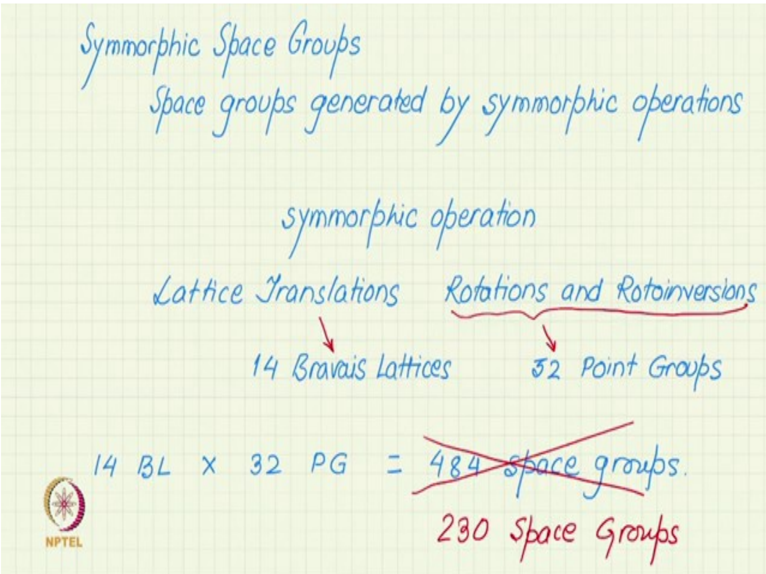

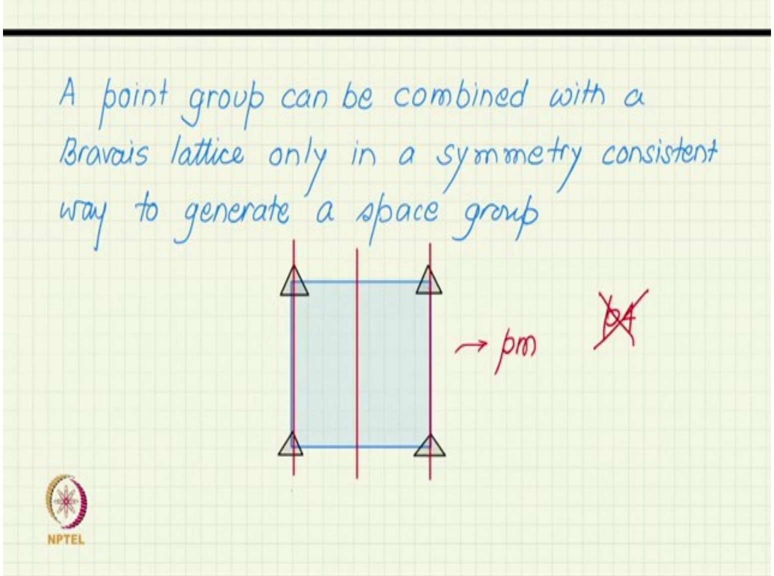

In this video we will discuss 73 symmorphic space groups. Remember when we were discussing the introduction to space groups we classified space groups into one of the classifications one of the possible classification of 3 dimensional space groups is in 73 symmorphic space groups and the remaining non symmorphic space group. We had defined symmorphic space groups in an earlier video but we will redefine it here and look at how do we get the 73 symmorphic space groups.

So, the definition of dimorphic space group is a space group which are generated only by symmorphic operations. So, recall that symmorphic operations are lattice translations, rotations and rotoinversions. So, what is left out in this it may look like that we have we are considering all operations translations, rotations and rotoinversions but no we are leaving out 2 important kinds of operations which are a screw and glide they are non symmorphic operations.

So, if we leave out those non symmorphic operations and generate a space group only by a symmorphic operations that is only by lattice translations, rotations and rotoinversions, and as you know rotoinversions include inversions and reflections. Now, if you look at the lattice translations so these actually determine 14 Bravais lattices. So, the different kinds of lattice translations which a lattice can have which a periodic pattern can have is classified into 14 Bravais lattices and we have also seen in detail that different kinds of rotations and rotoinversions form point groups and they can be classified into 32 point groups.

So, essentially that means that if we want to combine these to form our space groups we have to we have 14 Bravais lattices and 32 point groups to play with. So, it may appear that we can simply multiply these 2 numbers that 14 different kinds of lattices are there and we can combine them with 32 different kinds of point groups. So, we should be able to generate 484 space groups only this is not right and as we know that there are only 230 3 dimensional space groups.

So, what happens here why we do not get this number 484 and instead only a limited number of 230 space groups. So, this is because of an important requirement that a point group can be combined with a Bravais lattice only in a symmetric consistent way to generate a space group. Let me show you what does this mean. So, although we are now intending to discuss 3 dimensional space group but they still it is simpler for me to show this in a 2 d example which we have discussed in our plane group discussion in other videos but let me try to show you one simple case.

So, let me draw a square unit cell to this is a square unit cell representing a square lattice in 2 dimension suppose I put an object with 3-fold symmetry at the corners. So, the presence of these 3-fold symmetry triangles assume them to be collateral triangles, I have not been able to draw it very nicely. So, because of their presence, the 4 4-fold of the entire pattern is disturbed and is gone.

So, although I repeat these triangles in a square lattice I will not get a pattern with 4 4-fold symmetry. So, I will not call that a square space group, space group belonging to or plane group belonging to a square lattice. So, the squareness can be preserved only if we put objects which are consistent with the square symmetry. So, this is space group for example this plane group if my triangles are oriented this way will preserve the mirror planes but not the 4 4-fold and since the mirror planes are preserved and only one set of mirror planes are there, you know that we call this plane group as p m and it is not let us say it will not be p 4 or p 4 mm.

So, we do not generate new plane groups by putting an object with or object with a different point group than what is consistent with that particular 2 dimensional lattice. So, this also is true for the 3 dimensional case. So, we will always have to put objects which are consistent with the corresponding symmetry which the lattice represents to generate new space groups.

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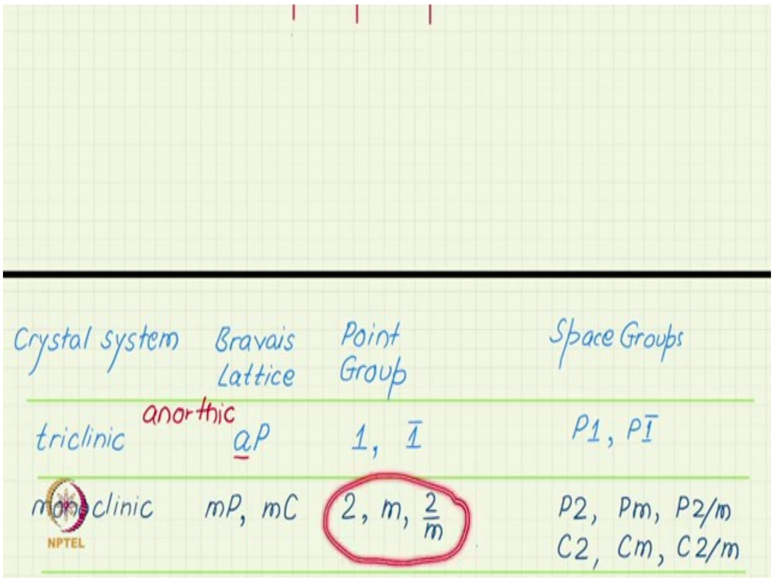

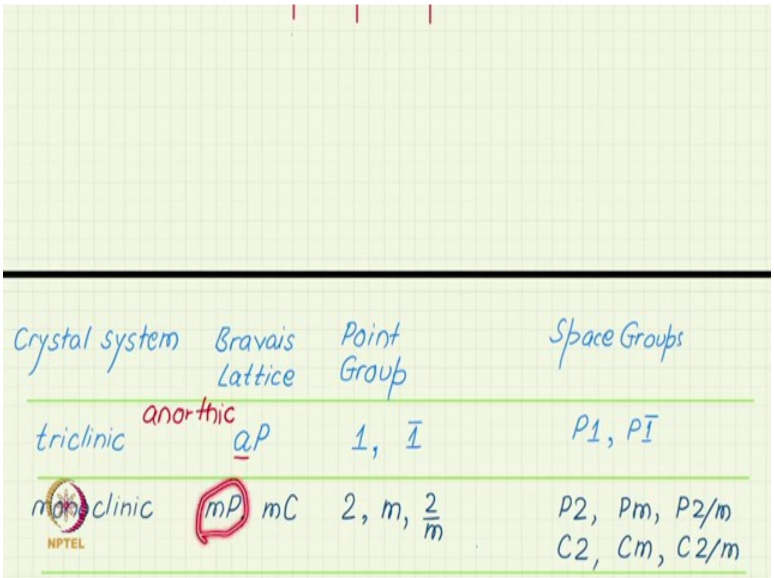

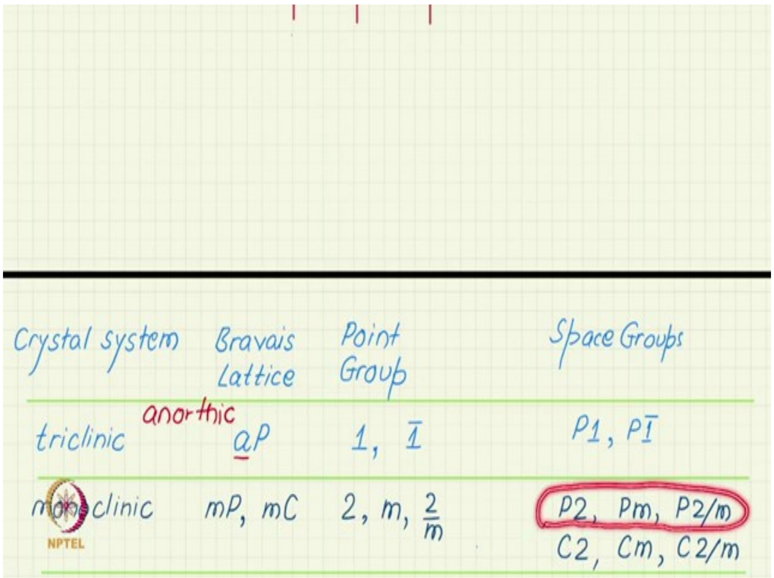

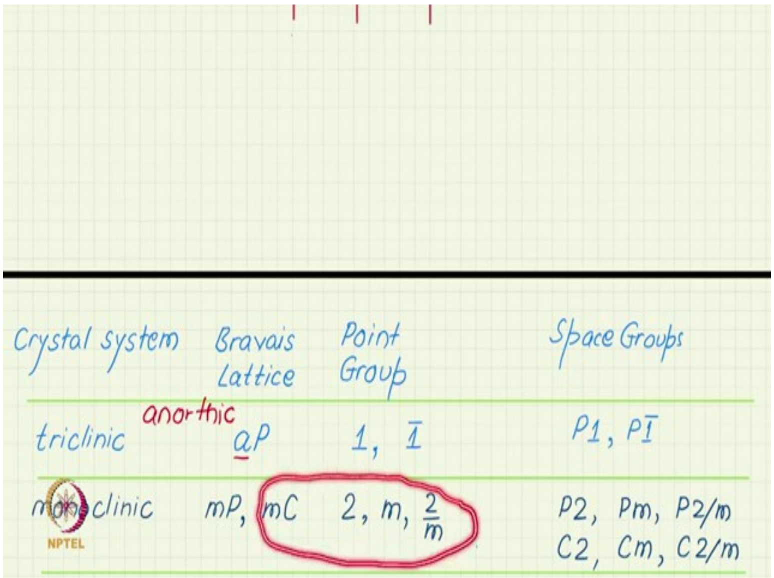

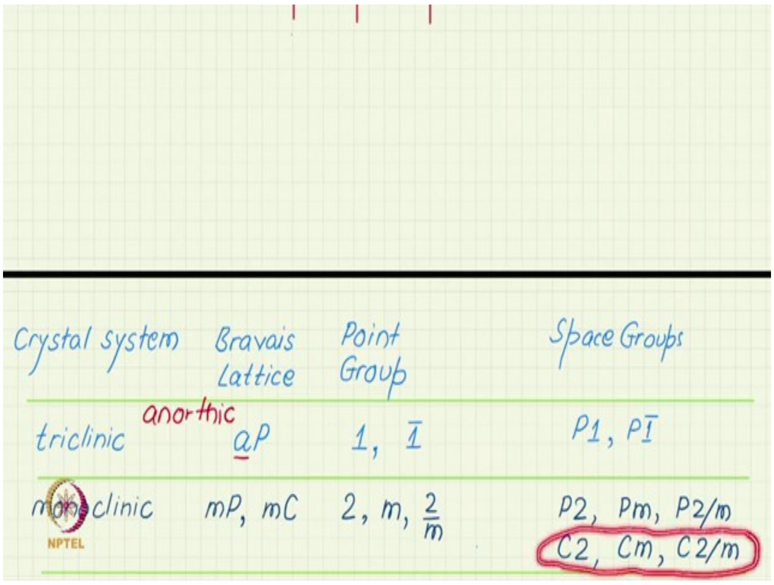

So, let us do that now one by one. So, for 3 dimensional case the symmetry of the lattice is classified into crystal systems. So, for example in the triclinic crystal system we have only one Bravais lattice which is the primitive triclinic, the triclinic symbol is a representing an orthotic and we have seen that in the triclinic system there are only 2-point group symmetries possible 1 and 1 bar identity or center of inversion.

So, only these 2 point groups are there and only one lattice is there. So, we can put these point groups to associate the objects with these point groups to the triclinic lattice the primitive triclinic lattice and that will generate 2 space groups for me who is Hermann Mauguin's symbols of P 1 and P 1 bar these are actually the first 2 space groups in the international table space group number 1 is P 1 and space group number 2 is P 1 bar.

Now, as we go down in this list suppose we consider the monoclinic crystal system it the required symmetry is a single 2-fold but it gives me 2 Bravais lattices monoclinic P primitive monoclinic and monoclinic C them and centered or base centered monoclinic. So, this will then give me and there are 3 point groups 2 m m, 2 by m. So, if I combine these point groups with m P I get the first row of space group p 2 p by m and p 2 by m and if I combine the m centered monoclinic with these 3 point groups I get another 3 space group in the second row C 2 C m and C 2 by m.

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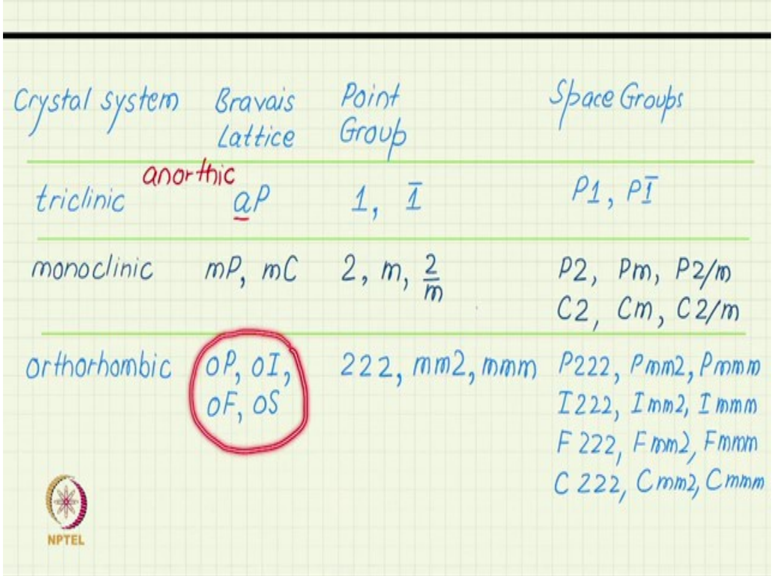

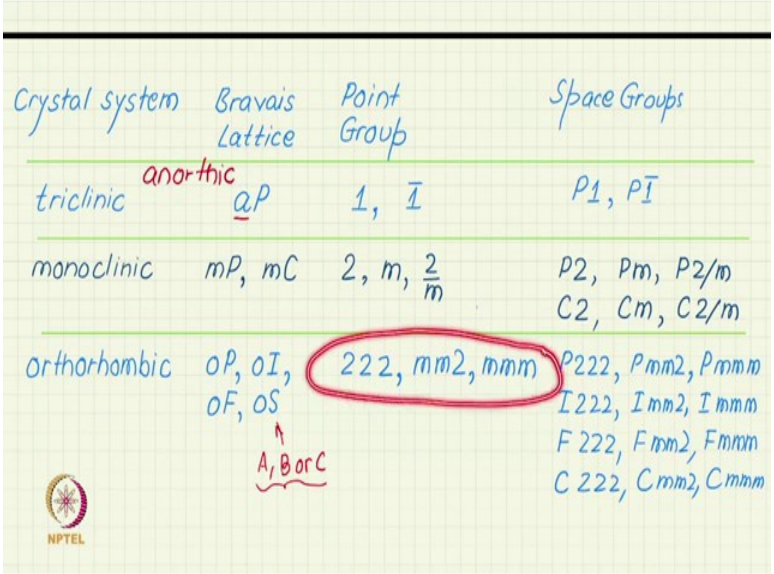

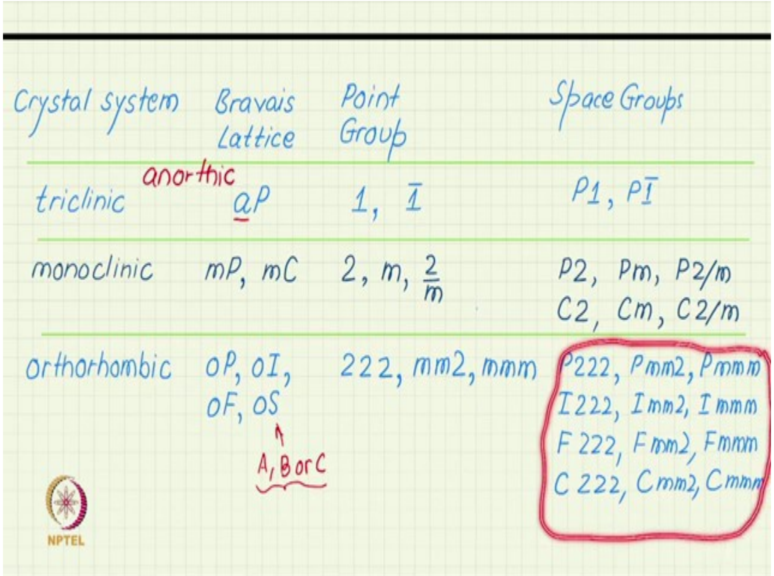

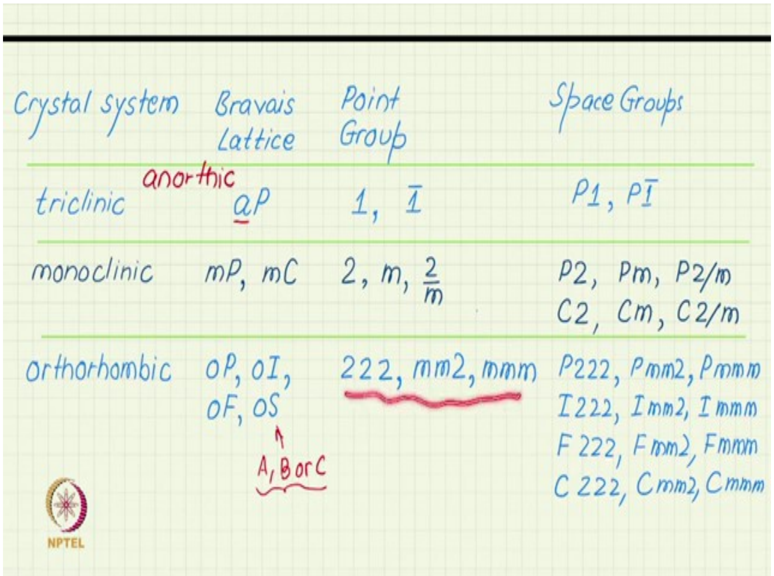

So, we continue this process with other crystal system. So, here is orthorhombic. So, you can see in orthorhombic we know that there are 4 lattices primitive body centered face centered and end centered S represents a general and centered which can be either A B or C. So, if we combine this 4 lattices and in orthorhombic system there are 3 point groups. So, 3 into 4 12 response groups you generate here. So, the primitive lattice with these 3 point groups will give P 2 2 P m m 2 and P m m m and so on.

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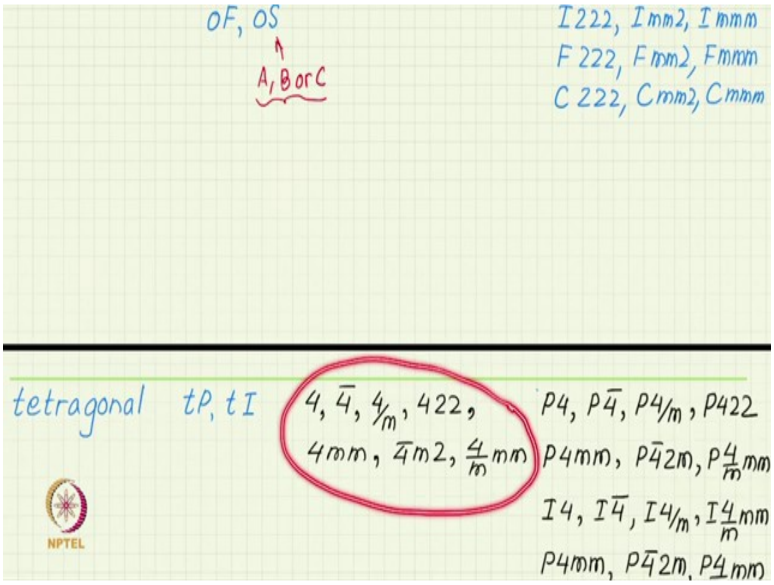

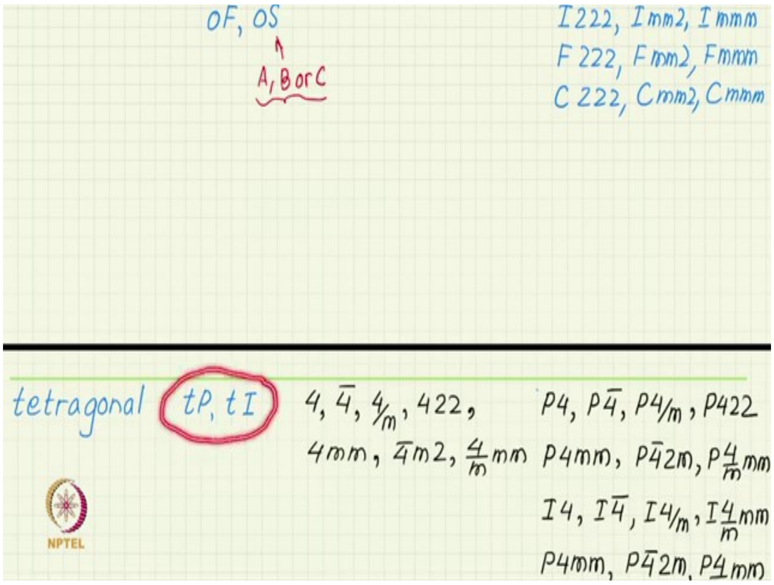

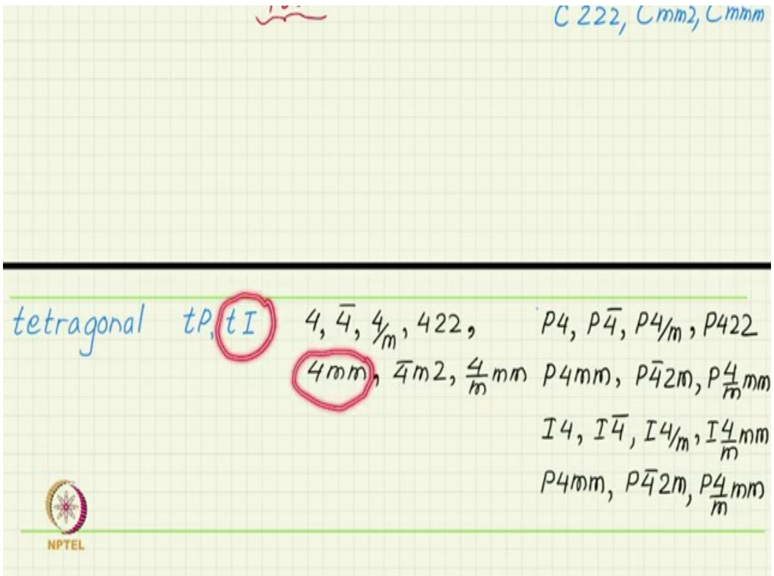

C 222, Cmm2, Cmmm

tetragonal   tP, tI $4, \bar{4}, 4/m, 422,$ $4mm, \bar{4}m2, \frac{4}{m}mm$

$P4, P4, P4/m, P422$

$P4mm, P\bar{4}2m, P\frac{4}{m}mm$

$I4, I\bar{4}, I4/m, I\frac{4}{m}mm$

$P4mm, P\bar{4}2m, P\frac{4}{m}mm$

C 222, Cmm2, Cmmm

tetragonal   tP, tI $4, \bar{4}, 4/m, 422,$ $4mm, \bar{4}m2, \frac{4}{m}mm$

$P4, P\bar{4}, P4/m, P422$

$P4mm, P\bar{4}2m, P\frac{4}{m}mm$

$I4, I\bar{4}, I4/m, I\frac{4}{m}mm$

$I4mm, I\bar{4}2m, I\frac{4}{m}mm$

C 222, Cmm2, Cmmm

tetragonal   tP, tI $4, \bar{4}, 4/m, 422,$ $4mm, \bar{4}m2, \frac{4}{m}mm$

$P4, P\bar{4}, P4/m, P422$

$P4mm, P\bar{4}2m, P\frac{4}{m}mm$

$I4, I\bar{4}, I4/m, I\frac{4}{m}mm$

$I4mm, I\bar{4}2m, I\frac{4}{m}mm$

Tetragonal has now 7 point groups required symmetry just single 4 4 or 4 bar that as we have seen in the analysis of 32 point groups gives us 7 tetragonal point groups. And there are 2 tetragonal Bravais lattices t P and t I. So, if I combine the 7 point groups with these 2 lattices I get 14 space groups which are represented here. So, for example, if I put 4 m m on an body centered tetragonal lattice I will get I i will get I 4 m m have I missed writing it.

I am writing less number of 4 P I have written all 7 for I have I think I made a mistake here let me correct that for you and for myself also this should not be repeated with P they should be repeated with I they just caught that mistake. So, let me fix this. So, I 4 m m, I 4 bar 2 m I 4 by m m m. So, as I was telling that if I put 4 m m point group on a t I lattice tetragonal body centered lattice, then I will get it 4 mm space group. So, similarly, for others.

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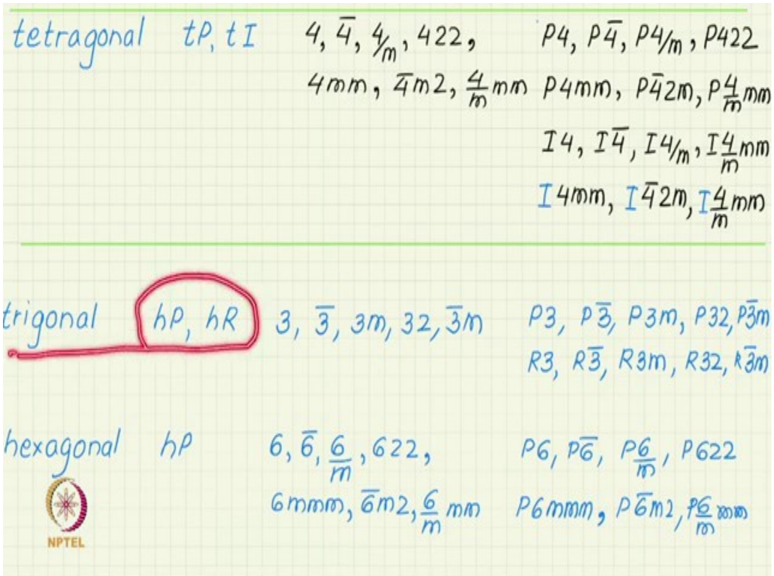

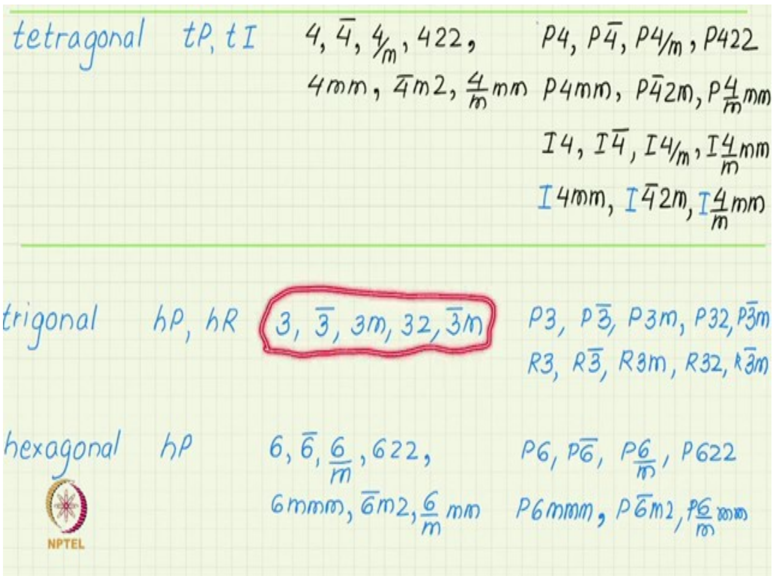

tetragonal	tP, tI	$4, \bar{4}, 4/m, 422,$	$P4, P\bar{4}, P4/m, P422$
		$4mm, \bar{4}m2, \frac{4}{m}mm$	$P4mm, P\bar{4}2m, P\frac{4}{m}mm$
			$I4, I\bar{4}, I4/m, I\frac{4}{m}mm$
			$I4mm, I\bar{4}2m, I\frac{4}{m}mm$
trigonal	hP, hR	$3, \bar{3}, 3m, 32, \bar{3}m$	$P3, P\bar{3}, P3m, P32, P\bar{3}m$
			$R3, R\bar{3}, R3m, R32, R\bar{3}m$
hexagonal	hP	$6, \bar{6}, \frac{6}{m}, 622,$	$P6, P\bar{6}, P\frac{6}{m}, P622$
		$6mmm, \bar{6}m2, \frac{6}{m}mm$	$P6mmm, P\bar{6}m2, P\frac{6}{m}mm$

tetragonal	tP, tI	$4, \bar{4}, 4/m, 422,$	$P4, P\bar{4}, P4/m, P422$
		$4mm, \bar{4}m2, \frac{4}{m}mm$	$P4mm, P\bar{4}2m, P\frac{4}{m}mm$
			$I4, I\bar{4}, I4/m, I\frac{4}{m}mm$
			$I4mm, I\bar{4}2m, I\frac{4}{m}mm$
trigonal	hP, hR	$3, \bar{3}, 3m, 32, \bar{3}m$	$P3, P\bar{3}, P3m, P32, P\bar{3}m$
			$R3, R\bar{3}, R3m, R32, R\bar{3}m$
hexagonal	hP	$6, \bar{6}, \frac{6}{m}, 622,$	$P6, P\bar{6}, P\frac{6}{m}, P622$
		$6mmm, \bar{6}m2, \frac{6}{m}mm$	$P6mmm, P\bar{6}m2, P\frac{6}{m}mm$

tetragonal	tP, tI	$4, \bar{4}, 4/m, 422,$	$P4, P\bar{4}, P4/m, P422$
		$4mm, \bar{4}m2, \frac{4}{m}mm$	$P4mm, P\bar{4}2m, P\frac{4}{m}mm$
			$I4, I\bar{4}, I4/m, I\frac{4}{m}mm$
			$I4mm, I\bar{4}2m, I\frac{4}{m}mm$
trigonal	hP, hR	$3, \bar{3}, 3m, 32, \bar{3}m$	$P3, P\bar{3}, P3m, P32, P\bar{3}m$
			$R3, R\bar{3}, R3m, R32, R\bar{3}m$
hexagonal	hP	$6, \bar{6}, \frac{6}{m}, 622,$	$P6, P\bar{6}, P\frac{6}{m}, P622$
		$6mmm, \bar{6}m2, \frac{6}{m}mm$	$P6mmm, P\bar{6}m2, P\frac{6}{m}mm$

Trigonal has 2 lattices, hexagonal, P and hexagonal R where I have another video which discusses this in detail. And there are 5 point groups 3, 3 bar, 3 m, 3 2 and 3 bar m. So, each of them combined with these 2 lattices give you the 10 point groups shown here.

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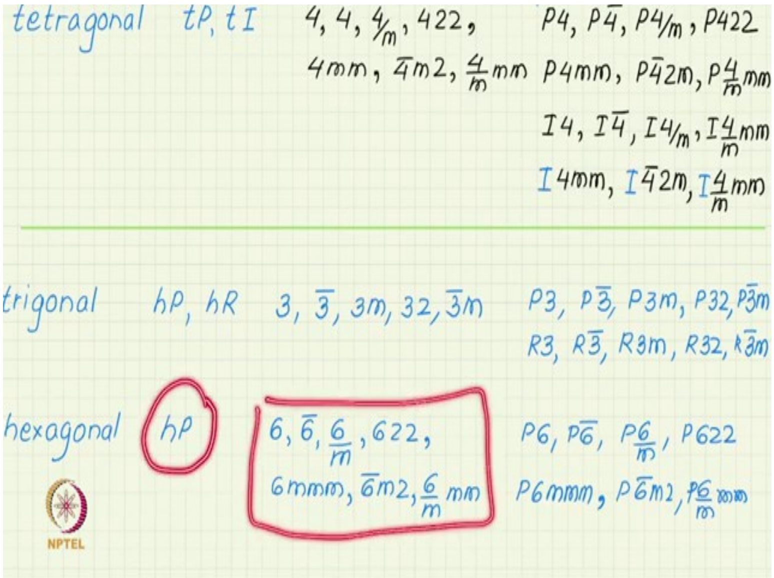

Hexagonal has again 7 point groups but there is only 1 lattice associated with hexagon, the hexagonal primitive. So, that generates the 7 point groups shown here.

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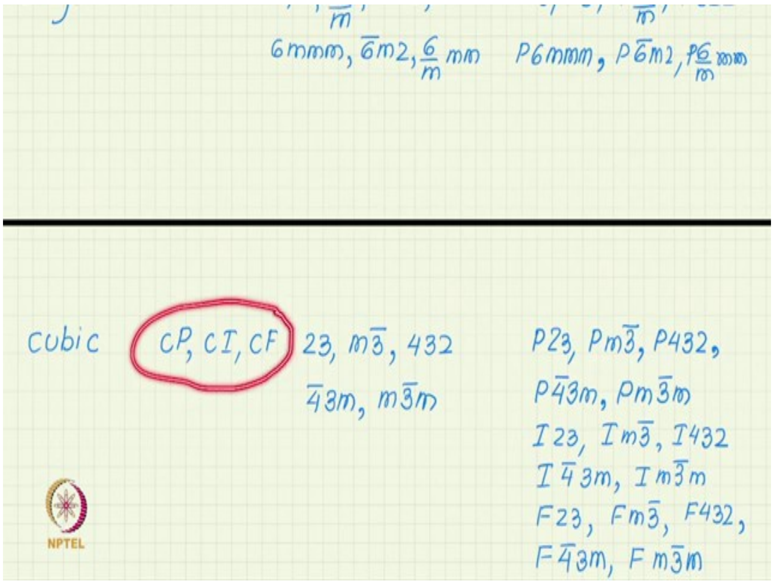


		$6mmm, \bar{6}m2, \frac{6}{m}mm$	$P6mmm, P\bar{6}m2, P\frac{6}{m}mm$

cubic	cP, cI, cF	$23, m\bar{3}, 432$, $\bar{4}3m, m\bar{3}m$	$P23, Pm\bar{3}, P432, P\bar{4}3m, Pm\bar{3}m$, $I23, Im\bar{3}, I432, I\bar{4}3m, Im\bar{3}m$, $F23, Fm\bar{3}, F432, F\bar{4}3m, Fm\bar{3}m$

cubic	cP, cI, cF	$23, m\bar{3}, 432$, $\bar{4}3m, m\bar{3}m$	$P23, Pm\bar{3}, P432, P\bar{4}3m, Pm\bar{3}m$, $I23, Im\bar{3}, I432, I\bar{4}3m, Im\bar{3}m$, $F23, Fm\bar{3}, F432, F\bar{4}3m, Fm\bar{3}m$

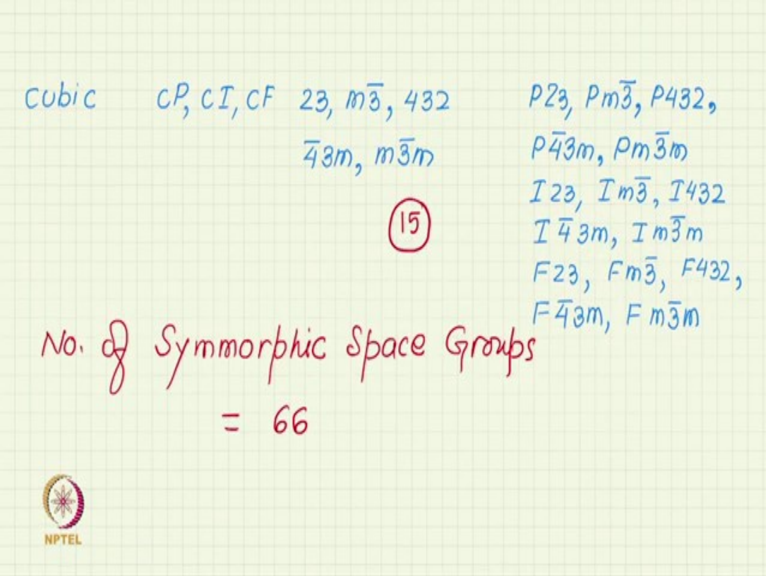
Crystal system	Bravais Lattice	Point Group		Space Groups
triclinic (anorthic)	aP	$1, \bar{1}$	2	$P1, P\bar{1}$
monoclinic	mP, mC	$2, m, \frac{2}{m}$		$P2, Pm, P2/m$, $C2, Cm, C2/m$
orthorhombic	oP, oI, oF, oS (A, B or C)	$222, mm2, mmm$		$P222, Pmm2, Pmmm$, $I222, Imm2, Immm$, $F222, Fmm2, Fmmm$

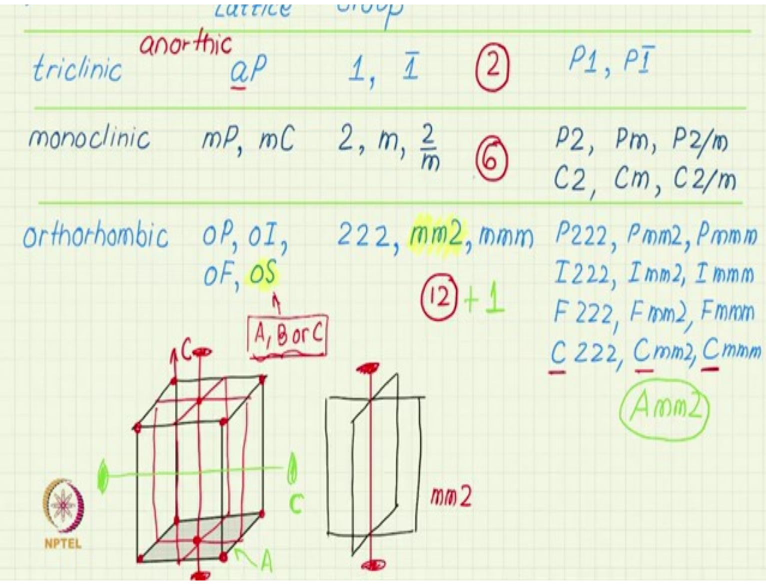
	Lattice	Group		
triclinic	anorthic aP	1, $\bar{1}$	2	P1, P$\bar{1}$
monoclinic	mP, mC	2, m, $\frac{2}{m}$	6	P2, Pm, P2/m C2, Cm, C2/m
orthorhombic	oP, oI, oF, oS A, B or C	222, mm2, mmm	12	P222, Pmm2, Pmmm I222, Imm2, Immm F222, Fmm2, Fmmm C222, Cmm2, Cmmm

			14	I4, I$\bar{4}$, I4/m, I$\frac{4}{m}$mm I4mm, I$\bar{4}$2m, I$\frac{4}{m}$mm
trigonal	hP, hR	3, $\bar{3}$, 3m, 32, $\bar{3}$m	10	P3, P$\bar{3}$, P3m, P32, P$\bar{3}$m R3, R$\bar{3}$, R3m, R32, R$\bar{3}$m
hexagonal	hP	6, $\bar{6}$, $\frac{6}{m}$, 622, 6mmm, $\bar{6}$m2, $\frac{6}{m}$mm	6	P6, P$\bar{6}$, P$\frac{6}{m}$, P622 P6mmm, P$\bar{6}$m2, P$\frac{6}{m}$mm

6

cubic	cP, cI, cF	23, m$\bar{3}$, 432 $\bar{4}$3m, m$\bar{3}$m	15	P23, Pm$\bar{3}$, P432, P$\bar{4}$3m, Pm$\bar{3}$m I23, Im$\bar{3}$, I432 I$\bar{4}$3m, Im$\bar{3}$m F23, Fm$\bar{3}$, F432, F$\bar{4}$3m, Fm$\bar{3}$m





And cubic you have 3 Bravais lattices primitive cubic, body centered cubic and face centered cubic, and you have 5 point groups you can generate 15 consistent Bravais lattices. So, 15 consistent space group. So, let us count the number how many we have got. So, this is 2 into 1. So, we have 2 here we have 6 in the monoclinic 4 into 3 12 in the orthorhombic. 7 into 2 so 14 in tetragonal 5 into 2 to 10 trigonal and 6 into 1 so 6 hexagonal and 5 into 3 15 cubic groups.

So, if you add all these numbers, 2 plus 6 plus 12 plus 14 plus 10 plus 6 and 15 you will get the number of space groups number of symmorphic space groups which we have generated is 66. However, as we noted in the title to this video, there are 73 space groups are 7 of them are still missing. So, where are the missing 7 because it seems we have already combined the point groups with the lattices in a consistent way. So, we should have got all of them but we have not got 7 of them are missing. So, let us look for the missing ones.

Now, when you come to orthorhombic lattice this this particular point group is interesting m m 2 and this particular lattice. That o S is all so interesting why they are interesting let us see for example in orthorhombic lattice when you have so this is my let us say orthorhombic unit cell and I am putting an object with m m 2 symmetry. Now m m 2 symmetry itself means that I have an m and I have another orthogonal m so there are 2 perpendicular mirror planes and the intersection of them is a 2-fold axis that is what is m by and m m 2 point group.

So, it has a unit 2-fold axis and if I look at the orthorhombic m centered orthorhombic and we have taken here for example, I told you that it can be either A B or C and here we have taken C as the example in the generation of a space group to C means if this is my C axis to C face it centered to the lattice points as shown by this red dot that means one face is centered and 1 pair of face is centered the other 2 pairs of faces the vertical faces are not centered.

Now, I can put my m m 2-point group in 2 possible orientations, either the 2-fold of m m 2 can be like this in which case the mirrors are mirrors are going this way. So, mirrors are parallel to the uncentered face of the unit cell. However, if I have tilt this and make the 2-fold pass this way, let me try to do it in a different color. If I take the green orientation of the 2-fold, then the mirror planes the 2-fold axis now is passing through an uncentered face.

So, because there is centered face and uncentered face, there are 2 possible orientations for the m m 2 object with m m 2-point group which can be placed in this lattice where it is 2-fold perpendicular to the centered phase or 2-fold perpendicular to uncentered phase if you place it the 2-fold in the uncentered phase then you generate a new space group and that will be called now since we prefer to call the centered we prefer to call the 2-fold direction as our C direction.

So, in the green case this will be my C phase. So, the centering is now no more in on the C phase. So, this will be called in that case and A phase. So, the centering is now A center A m m 2. So, we generate a new point group because of this different orientation A m m 2, and we create one new space group. So, this is one of the 7 missing ones.

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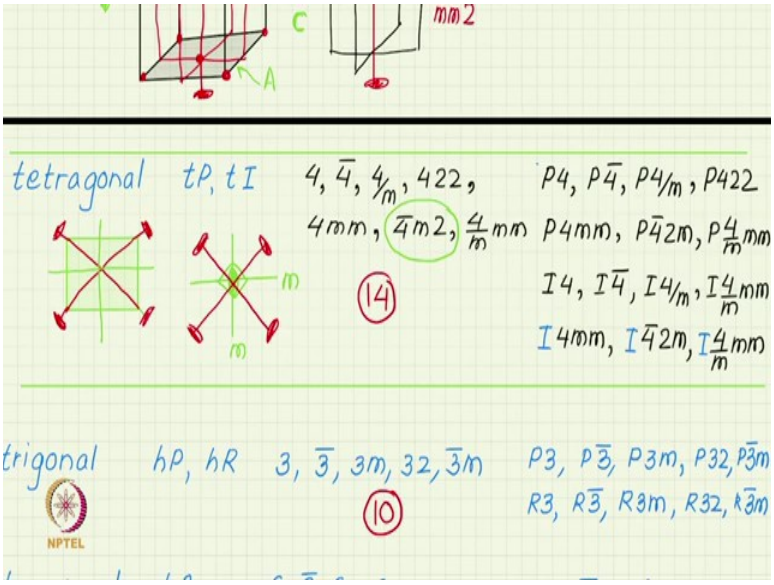

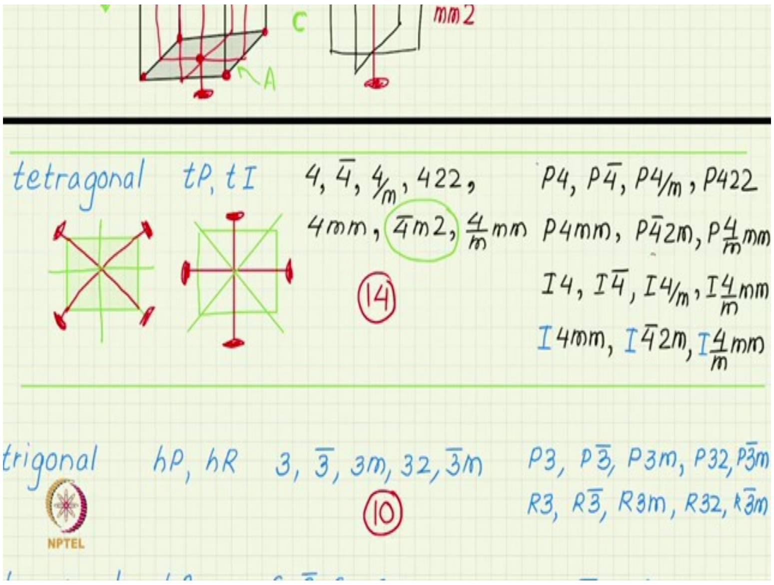

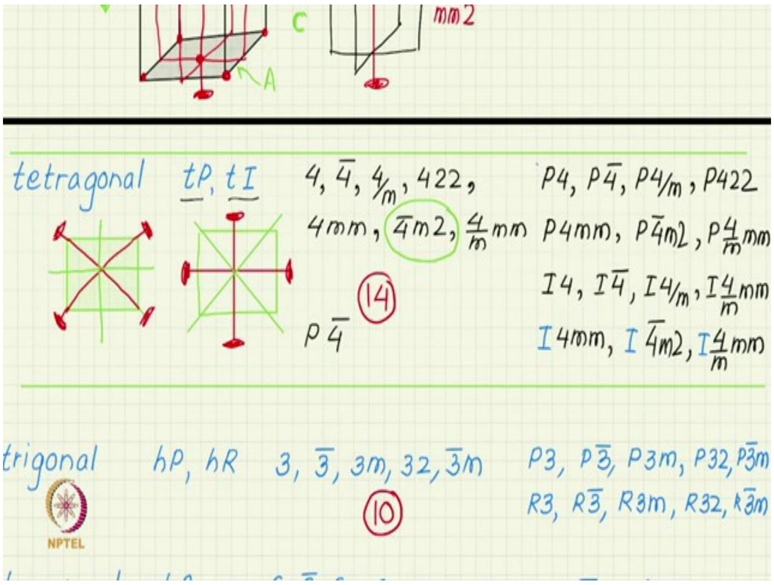

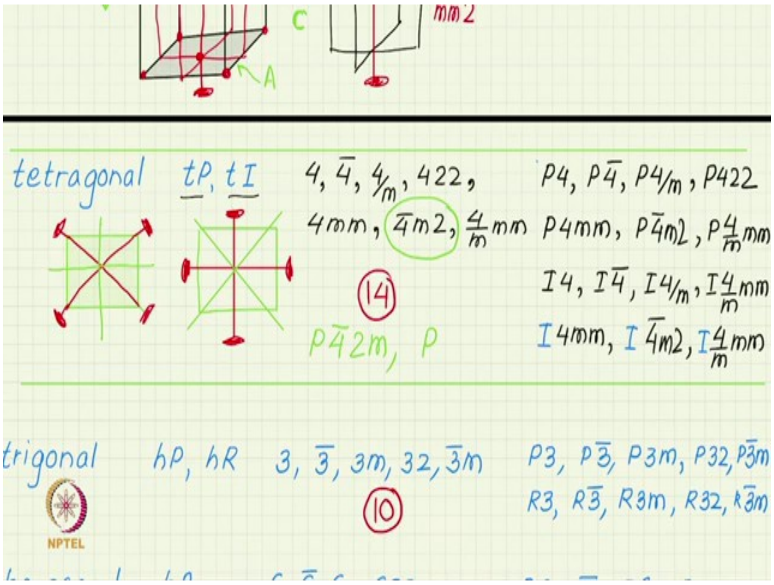

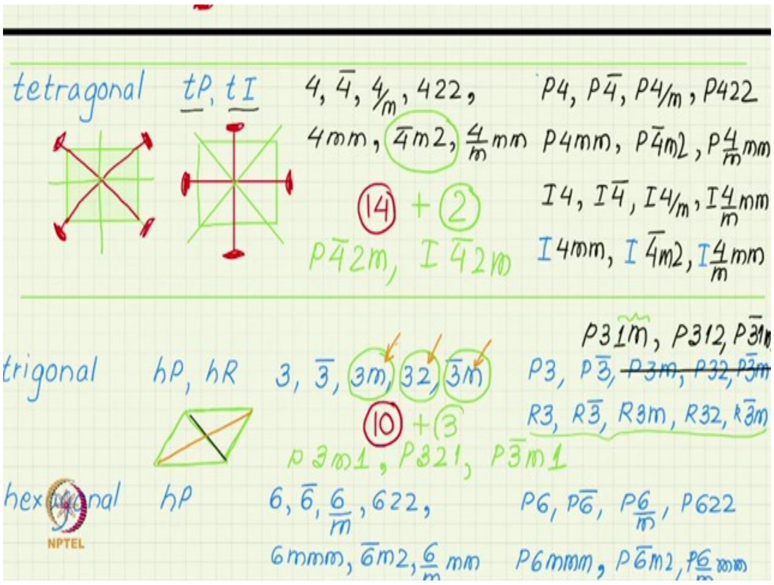

In tetragonal similar situation comes with the point group 4 bar m 2. So, in tetragonal let me draw the square face of the tetragonal and in the 4 bar m 2 plane group sorry in the 4 bar m 2-point group, there are mirror planes where is 4 bar in the center. If you recall the development of 4 bar m 2 which is discussed in detail in another of my video. Then you will find that it has 2 perpendicular mirrors as well as 2 perpendicular 2-folds.

Now, this can be placed exactly in this orientation such that the mirror planes mirror planes are parallel to the cube edge sorry the mirror planes are perpendicular to the edges of the unit cell the square edges of the unit cell and the 2-folds are along the diagonal 2-fold are along the diagonal but you can of course imagine another orientation possible I have out of space let me clear this and create another little square and in this case I will now put the 2-fold along the square edges parallel to the square edges whereas mirrors in the perpendicular direction.

So, you can see this is actually the same point group but oriented differently with respect to the lattice. And because of this difference in orientation the symmetry because the space group captures not just the individual symmetry elements but their interrelations also. So, the way the mirror planes and 2-fold axis are related to the translational symmetry are different in these 2 cases. So, you will generate different point groups if you place it in this different way.

So, one of them will be called 4 bar m 2 see I have already mixing up the notation. So, I have written here 4 bar m 2 but here I wrote 4, 4 bar 2 m. So, maybe I should have written originally I should have written let me try to fix that I was not being very careful that is a good learning for you also that in this point group one has to be careful in both cases let me write whatever I had written initially 4 bar m 2, 4 bar m 2 but now for both the lattices the primitive and the body centered I generate 2 more space groups by putting it in a different orientation and that is described by writing m and 2 in a different sequence.

So, I have now I have P 4 bar 2 m and P sorry I 4 bar 2 m the 2 new space groups get created in the tetragonal in the trigonal in the plane group also we had seen that actually the 3 m, 3 m has a single mirror 3 2 has a single mirror and 3 bar m has a single mirror whereas, the lattice has a rhombus base which has a short diagonal let me say a short diagonal the black diagonal or the long diagonal which is a goal diagonal these 2 directions are not symmetry equivalent.

So, the question is whether I am placing the mirror in 3 m m, 3 bar m or the 2-fold in 3 2 along the short diagonal or the long diagonal depending on that you will get 2 different kinds of space groups. So, really here this is not a complete description of the space group this is not how an international table they will be given. But they will like to specify clearly that along which direction the mirror or 2-fold is aligned.

So, in one case it will be written notes P 3 1 m, P 3 1 2 and P 3 bar 1 m and in the other case, it will be written as P 3 m 1. So, m m 1 and 1 m m. So, they are changing place and by the changing of place different space group is getting created P 3 2 1 and P 3 bar m 1. So, you can see that 3 different space groups new space groups are generated based on whether the mirror or 2-fold in these 3 point groups are aligned along the short diagonal or long diagonal of the unit cell.

So, this issue does not come with the rhombohedral case because it has there the mirrors and the 2-folds can be placed only in a unique way this freedom is not there to place them either along one direction or the other direction. So, you get here 3 new space groups.

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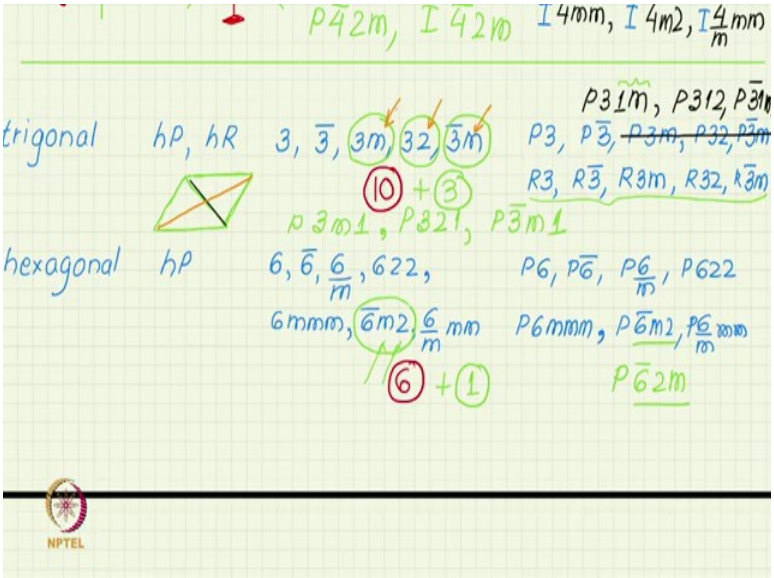

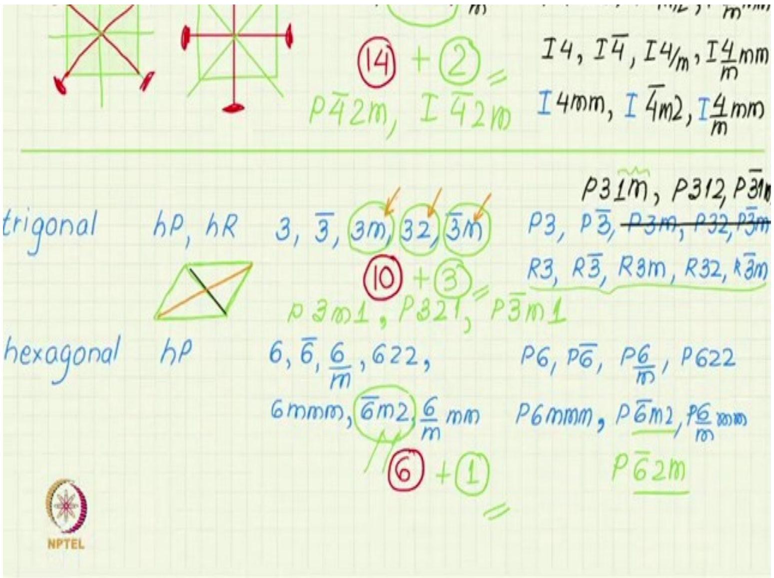

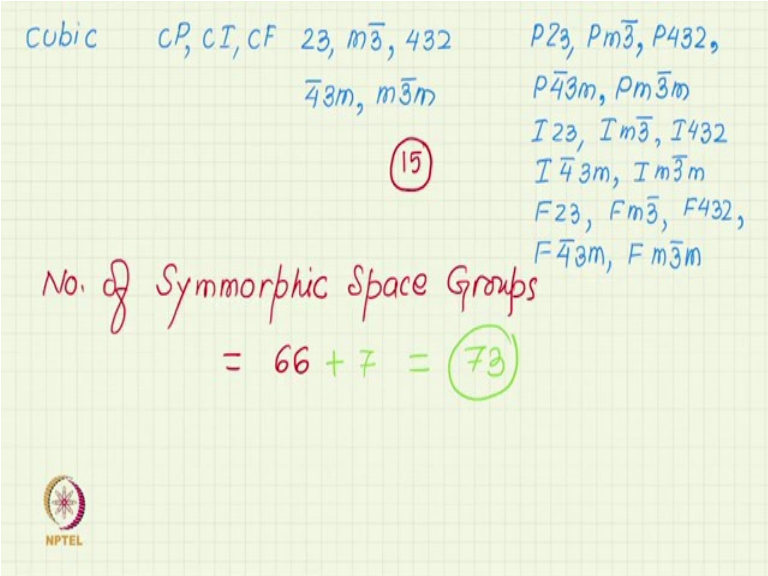

Now, we have gone to a lot of details in the hexagonal the same issue comes with 6 bar m 2, because there is a mirror and there is a 2-fold and they can be aligned either along the short diagonal or along the long diagonal. So, here also you will generate one more space group, which we will now call P 6 bar 2 m. So, it is 6 bar m 2 other orientation will be 6 bar 2 m.

So, with all this hard work we have now probably found all the missing ones, 1 plus 2 3 plus 3 6 and 1 7. So, 66 plus 7 is equal to 73 symmorphic space groups we have found and listed here in their symbols.

Of course, we are only giving the Hermann Mauguin's symbol of the space groups we have not and we have looked at little bit of their symmetries the entire details symmetry one has to look up in the international tables. And we do not have time to look in the entire details. But what I have tried to explain you that how does this number 73 for symmorphic space groups arise. Thank you very much.