3D Space Groups XIV Interpretation of International Table Page
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Lecture-25d
Part 7: Generators Selected

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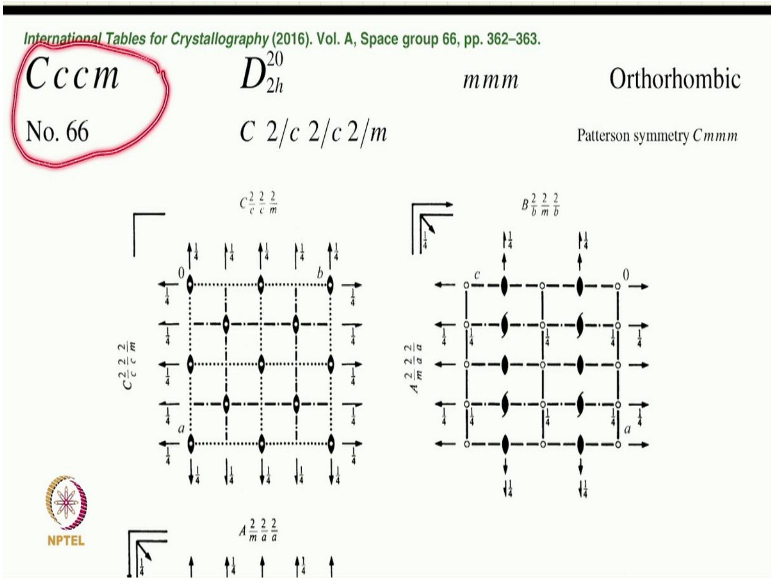
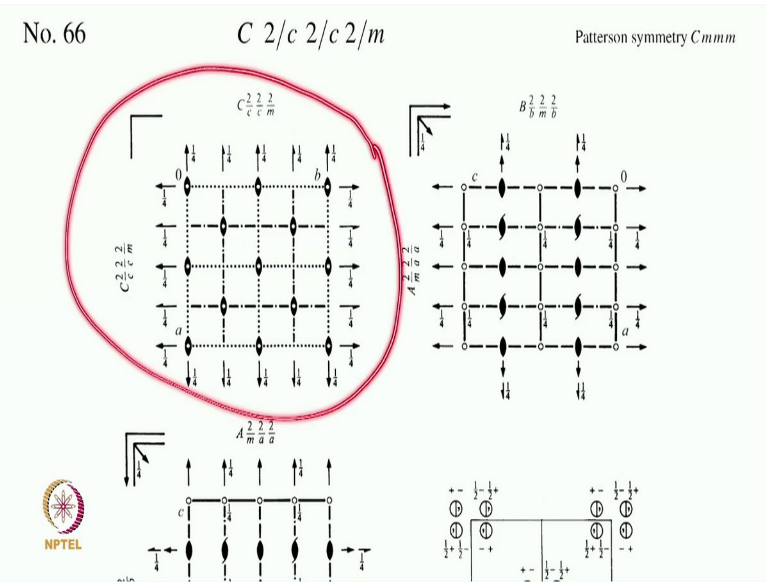
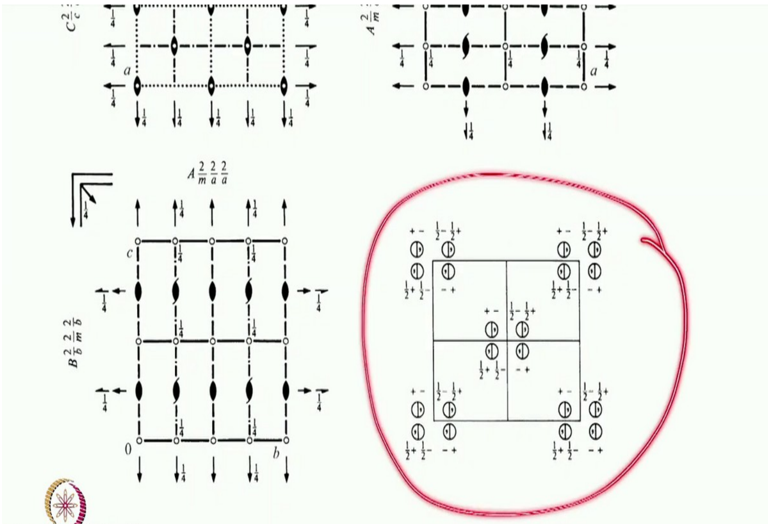
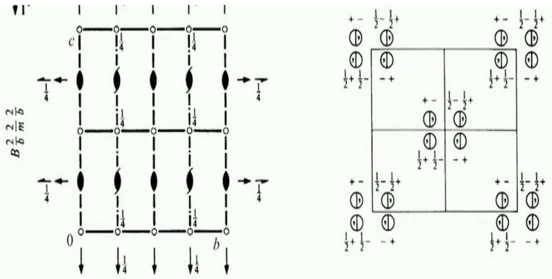






n at centre (2/m) at $cc2/m$

metric unit $0 \le x \le \frac{1}{4}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$



Origin at centre $(2/m)$ at $cc2/m$

Asymmetric unit $0 \le x \le \frac{1}{4}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$

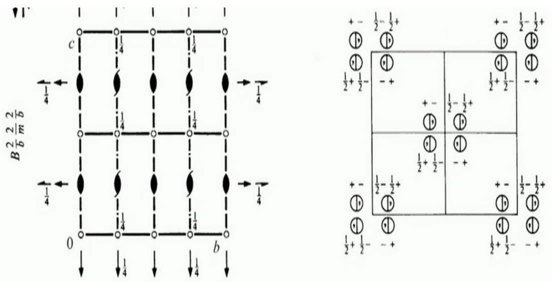
Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) 2 $0,0,z$	(3) 2 $0,y,\frac{1}{4}$	(4) 2 $x,0,\frac{1}{4}$
(5) $\bar{1}$ $0,0,0$	(6) m $x,y,0$	(7) c $x,0,z$	(8) c $0,y,z$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$	(2) 2 $\frac{1}{4},\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},\frac{1}{4}$
(5) $\bar{1}$ $\frac{1}{4},\frac{1}{4},0$	(6) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,0$	(7) $n(\frac{1}{2},0,\frac{1}{2})$ $x,\frac{1}{4},z$	(8) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,z$



Origin at centre $(2/m)$ at $cc2/m$

Asymmetric unit $0 \le x \le \frac{1}{4}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1 (2) 2 $0,0,z$ (3) 2 $0,y,\frac{1}{4}$ (4) 2 $x,0,\frac{1}{4}$
(5) $\bar{1}$ $0,0,0$ (6) m $x,y,0$ (7) c $x,0,z$ (8) c $0,y,z$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$ (2) 2 $\frac{1}{4},\frac{1}{4},z$ (3) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,\frac{1}{4}$ (4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},\frac{1}{4}$
(5) $\bar{1}$ $\frac{1}{4},\frac{1}{4},0$ (6) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,0$ (7) $n(\frac{1}{2},0,\frac{1}{2})$ $x,\frac{1}{4},z$ (8) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,z$

Welcome to this seventh part in our series of Interpretation of international tables page, in this part, we will look at the generators selected. So, if we actually look at the table which we were looking at in particular, this page group number 66 Cccm. And we have looked at the first page in detail by now, the symmetry element diagram, the general position diagram, then the selection of origin, the asymmetric unit and finally, the symmetry operations.

Now, let us look at let us continue because this is only half of the information half the table for this particular space group, some of the space groups are contained in only one page of the International tables, but some of them is spread into 2 pages and some even more than 2 pages, this particular space group is described in 2 pages. So, let us look at the contents of the seven second page now.

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CONTINUED No. 66 *Cccm*

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates $(0,0,0)+ \quad (\frac{1}{2},\frac{1}{2},0)+$				Reflection conditions
					General:
16 m 1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}+\frac{1}{2}$	(4) $x,\bar{y},\bar{z}+\frac{1}{2}$	hkl: $h+k=2n$
	(5) $\bar{x},\bar{y},\bar{z}$	(6) $x,y,\bar{z}$	(7) $x,\bar{y},z+\frac{1}{2}$	(8) $\bar{x},y,z+\frac{1}{2}$	$0kl$: $k,l=2n$
					$h0l$: $h,l=2n$
					$hk0$: $h+k=2n$
					$h00$: $h=2n$
					$0k0$: $k=2n$
					$00l$: $l=2n$
					Special: as above, plus
8 l . . m	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{x},y,\frac{1}{2}$	$x,\bar{y},\frac{1}{2}$	no extra conditions
8 k . . 2	$\frac{1}{4},\frac{1}{4},z$	$\frac{3}{4},\frac{1}{4},\bar{z}+\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},\bar{z}$	$\frac{1}{4},\frac{3}{4},z+\frac{1}{2}$	hkl: $k+l=2n$
8 j . . 2	$0,\frac{1}{2},z$	$0,\frac{1}{2},\bar{z}+\frac{1}{2}$	$0,\frac{1}{2},\bar{z}$	$0,\frac{1}{2},z+\frac{1}{2}$	hkl: $l=2n$

The second page begins with continued which means that it is the continuation of the same space group number 66. And then, we look at the next item in the list is the Generators selected this is an important concept and we will look at the meaning of this generators selected. So, let me try to cut and paste the generator selected along with the symmetry operations.

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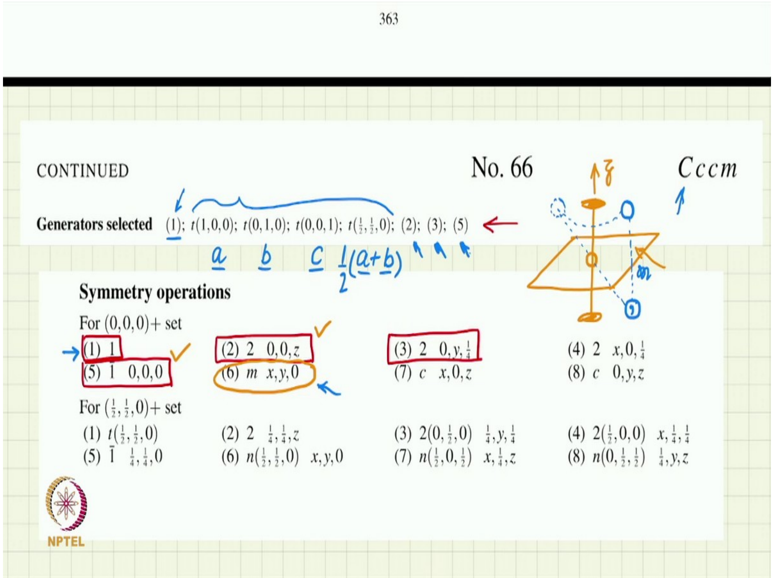

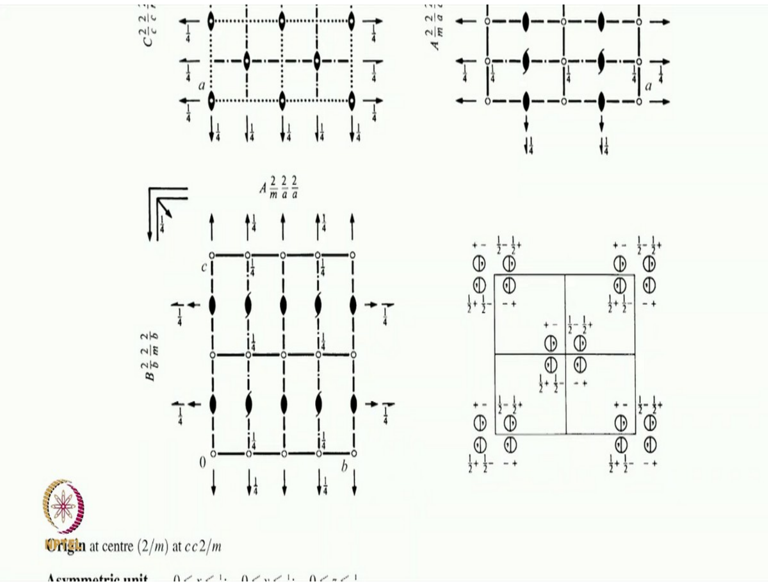

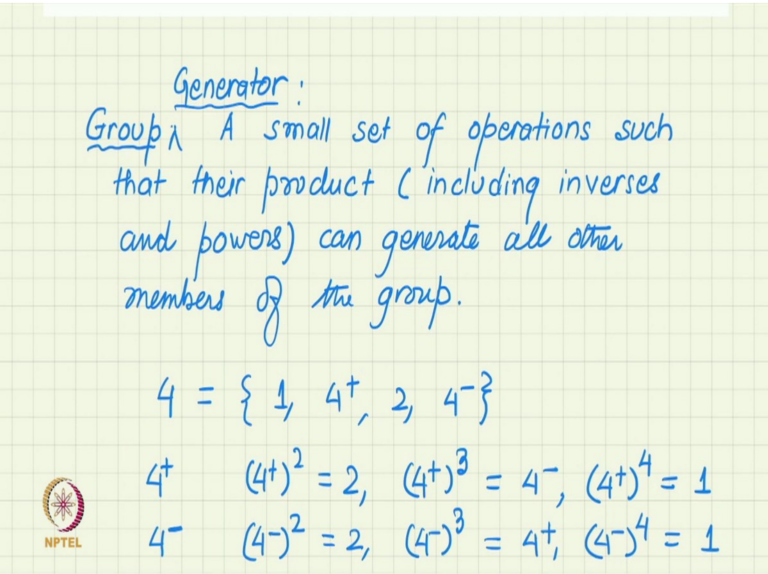

So, before we start with just a general introduction, which we have looked at in some of the previous videos, that any group, generator is a property of a group. So, for any group you can select a small set of operations such that their combinations and when we say combinations means, we mean the group product so, let me write it as products there so, what I am defining is not group but group generator.

So, group generator is a small set of operations from the group such that their product and when we say their product, it should also include including inverses and powers, can generate all other members of the group so, every member of the group can be written as a product of a finite set of operations from the group.

So, then it is called a group generator a very simple example, let us consider the point group 4, point group 4 has 4 operations 1, 4 plus, 2 and 4 minus. But if we just consider the element 4 plus. Then all other operations I can write as a product or power of 4 plus for example, you know that 4 plus square will be 2, 4 plus cube will be 4 minus and 4 plus to the power 4 will be 1.

So, you can see that all operations of this group point group can be generated by the operation 4 plus. So, 4 plus can represent is a generator of this group, the generator of a group are not unique. So, for example, in this case I selected 4 plus, but you can convince yourself that if I had selected 4 minus that is instead of a counterclockwise rotation by 90 degree, if I select clockwise rotation by 90 degree, this will also generate all the operations.

So, for example, 4 minus square is 2, 4 minus cube will now become 4 plus and 4 minus to the power 4 will again give me an identity. So, either 4 plus or 4 minus can be selected as generator of this group.

In fact, it is not even necessary that the generator the set of generators be minimal, sometimes for convenience and for some other additional aspects in mind that how you want to use those generators, you can select a generator, which is not really a minimal set.

So, for example, I say that 4 plus is the generator of the group obviously, if I take both 4 plus and 2, that will also be a generator. So, 2 itself gets generated by 4 plus. So, I need not have kept it in my generator, but it is allowed mathematically and sometimes people use that sort of generator also.

Generator is particularly important for space group, because unlike point group, point groups are finite group, I have taken an example of a very small group which has an order 4, only 4 operations, but in particular the space group is an infinite group, because the translation space group contains translations and translations are infinite. Infact, translation themselves form a subgroup of the space group and this subgroup itself is infinite of infinite order.

So, there are infinitely many symmetry operations in the space group. So, there it is useful to have a small set of generators, so, you can find a small set of generators, which will generate all these infinitely many operations and this is what is given a selection is given by the International Table other selections are possible, but one is specific selection one recommended selection of generators is given by this line in the second page, top of the second page generator selected.

And these are the generators which are selected for this particular group, Space group number 66. So, some of them are just serial numbers. And that is why I have kept the symmetry operations block also here close by to refer to. So, these serial numbers are actually referring to the operations given by these numbers.

So, for example, 1 is the identity operation then, there are 3 are other 4 translations, t represents translation. So, you have 1 0 0 which is the a translation 0 1 0 which is the b translation, 0 1 c translation and finally, since it is a C centered lattice, you need a centering translation of half half 0, so, that is you can say half of a plus b. So, that is the final translation.

So, these 4 translations are selected as part of the generator and then there is an identity and 3 other point operations or 3 other operations, symmetry operations are selected as part of this generator. So, those are given by their serial numbers. So, what is selected is 2.

So, 1 is selected, 2 is selected, then 3 and 5, that means along with the 4 translations which have been selected. Along with those 4 translations, if you select the 2 fold axis number 2, a 2 fold rotation around the z axis, the number 3 a 2 fold rotation about y axis, not really y axis, but parallel to the y axis, but at a height 1 4, which is the z value there and finally, the number 5, which is a center of inverse.

So, these 4 translations, and 4 of these operations 3, 3 symmetry operations listed here. And finally, 1, which is the identity operation identity really, if you think is not really necessary for selecting in the group, because identity leaves the operation unchanged. So, even if we drop the identity, we will still have the generators, but for for some mathematical reason the international tables have decided to keep identity also as part of the generator, particularly to relate the group to its subgroup.

Because finally, identity is a subgroup of all space groups, identity alone is the space group. So that is p 1, p 1 is a space group, where the only operation apart from translations is the identity operation. So, by convention, the first generator selected is always the identity and then it follows by translations and then other significant useful symmetry operations are selected as generator.

So, what about the symmetry operations which have been left out? Well, as we have said, the property of the generator is that any operation of the group can be written as product of operations from the generator.

So, since we here we have selected only these generators, these operations as the generator, any other symmetry operation, which is not part of the generator, can be written as a combination of these other operations. So, let me take one of the simplest example number 6. Number 6 is not listed as generated, but this is a mirror plane in the xy plane.

But a 2 fold operation along z-axis is selected, inverse and center in the origin is selected. And you know very well, from your study of symmetry, that if you have a 2 fold axis in this case along the z-axis and if you have a mirror plane, sorry, if you have an inversion center, if you have an inversion center.

Let me try to draw it in small open circle, which is, what is the international symbol you will see in our diagram. The inversion centers are shown by open circles. So, that open circle representing inversion center, so the combination of 2 fold with the inversion center is a mirror, like we tried to show it with a smallest schematic.

So, I start with this object, I rotate it by 180 degree about the 2 fold. So, that is the 2 fold rotation that will take me there and then I inverted in the inversion center. So it will come here with a chain handedness. And you can see that these 2 objects are related by a mirror. And that is exactly the mirror 6, which is shown here mirror in the xy plane.

So, 6 was not part of the generator, but it can be produced as product of 2 other operations in the generator. Similarly, all other operations which are listed here, which are not listed in the generator, can actually be produced as product of the generator. I leave this as an exercise for you. You can try as many of them as you like. Thank you very much.