3D Space Groups XII:
Interpretation of International Table Page
Part-5: Asymmetric Unit
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Lecture 25 b

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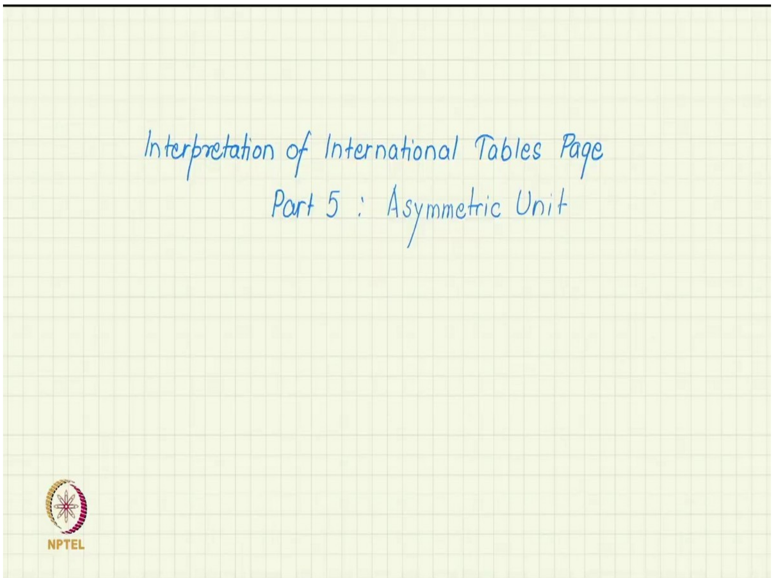

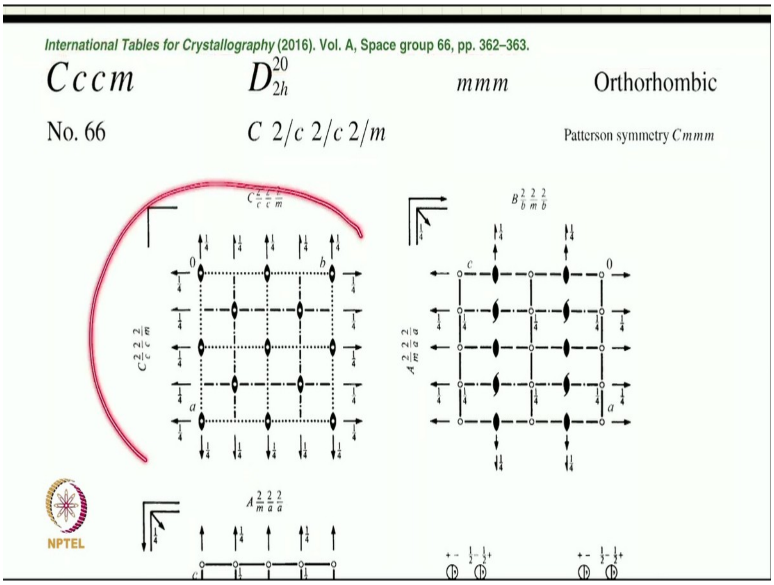

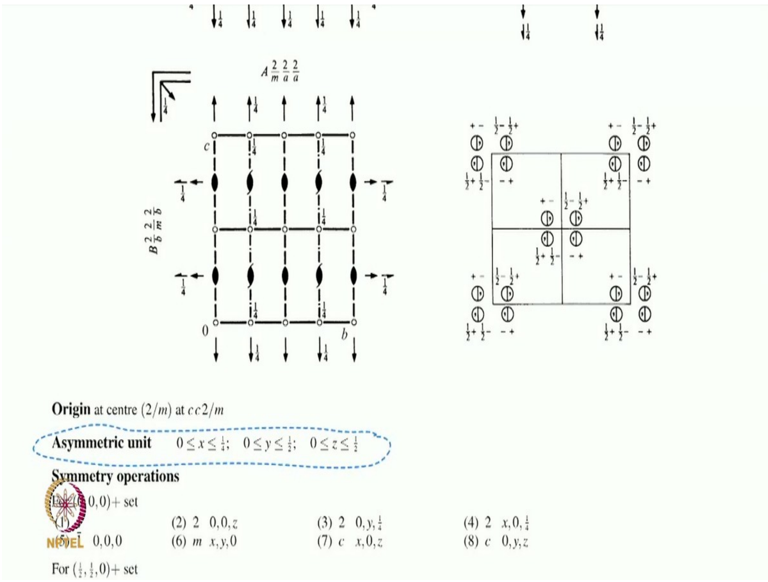

We now come to part 5 of our International Table page interpretation and in this part, we will look at asymmetric unit. So, you can see there is a space group we have been looking at, space group number 66. We look at the header information then we look at the symmetry element diagram, the general positions diagram and we looked at origin. So, the next item is this asymmetric unit. So, let us look at this asymmetric unit.

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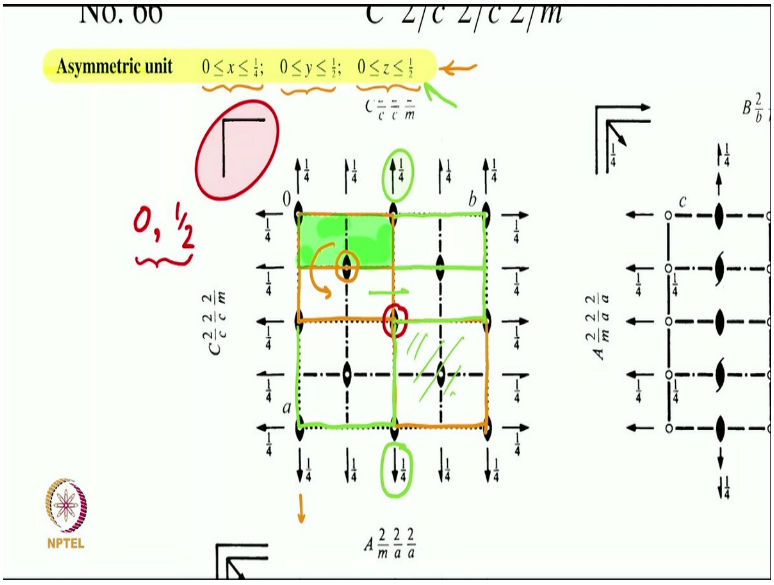

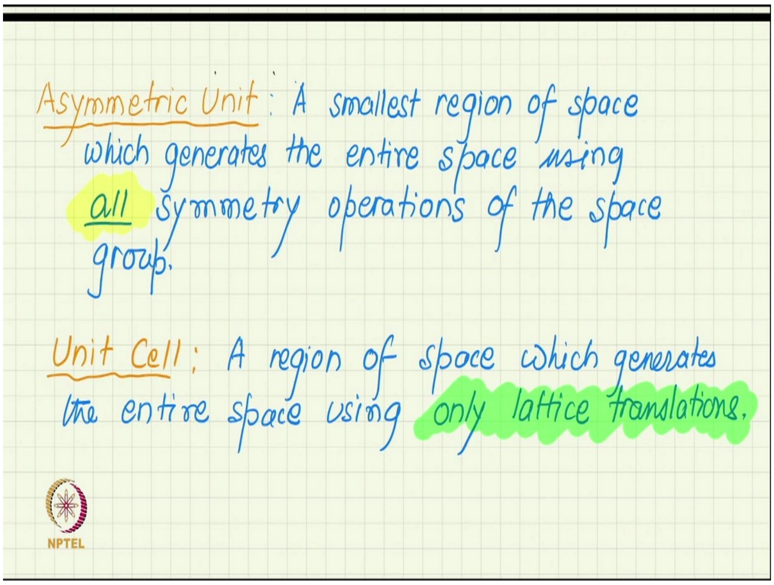

So, let me do a little cut and paste job let me put the asymmetric unit information here. So, this is our asymmetric unit. What is the definition of asymmetric unit? Let us first define a symmetric unit. So, as asymmetric unit is a smallest region of space which generates the entire space using all symmetry operations of the space group. So, the order needs to be emphasized we are using all symmetry operations and this is what distinguishes it from unit cell. So, let us define unit cell also, in unit cell is a region of space which generates or you can say covers the entire space using only lattice translations.

So, only lattice translations this is what is the difference between unit cell and asymmetric unit. In unit cell we are restricted to only translate the volume the unit cell volume to fill a space. In asymmetric unit we use all symmetry operations of the space group. So, along with translation, we can rotate or reflect the volume if the symmetry operations are available in the space group. So, let us look at the example with which we are working. So, here is our asymmetric metric unit defined for this particular space group.

So, what is given here is actually the boundaries of the asymmetric unit cell. So, you can see that x varies from 0 to quarter. So, x axis is downwards, and it is varying from 0 to quarter. So, in the x axis, we are going 0 to quarter. So, we will go only up to this much, in the y axis, we are going 0 to half. So, we go there. So, the projection of the asymmetric unit cell in the x y plane in the ab plane becomes this, this little box and you can see that in the z, we are going 0 to half.

So, you can imagine a prism or a parallel pippin based on this, this base and of a height equal to half the height of the unit cell. So, that region that domain becomes the asymmetric unit.

So, let me try to highlight this to large. So, between these golden borders filled with this green color is my asymmetric unit. So, you can see that the unit cell is very long, the unit cell is that entire rectangular box which is drawn. So that is the unit cell, but the asymmetric unit is much, much, much smaller than the unit cell.

Now, how is it that this region will fill that space using the symmetry operations of the space group. So, let us look at that. So, let me first use this 2-fold, the 2-fold which I have circled right now. So, if I rotate this volume, the green volume, the asymmetric unit about this 2-fold, which is going tangentially to the front face of the asymmetric unit, then the rotated asymmetric unit will fill this space, you can convince yourself that the rotated thing, if you rotate this about that 2-fold, then you will fill this region.

Now, you will see that there is another 2-fold now, I am circling it in red and if I rotate this now, bigger box equal to the 2 asymmetric unit about this 2-fold then you will get you will fill this region of space. So, you have filled half of the area, which is seen in the projection, but too little squares on the right and on the left are still left and how do we fill that region. So, there are symmetry operations available in this space group. So, let us look at this 2-fold axis which I have just circled in green at a high one forth. This 2-fold axis is also going tangential to the one of the boundaries of the asymmetric unit, it is going to the right boundary of the shaded asymmetric unit my original asymmetric unit.

And if you rotate this asymmetric unit I have to be careful, let us see that to see that we have defined the difference between a symmetric unit and unit cell. So, I should not be calling the asymmetric unit as my unit cell. So, the asymmetric unit. So, if you rotate this green asymmetric unit about this 2-fold at quarter, then you will fill the adjacent space. Let me show it in green. The green asymmetric unit when rotated about one forth, I had 2-fold will fill this particular space. And similarly, this one, this one will rotate here.

So, you will fill this entire volume. And that same 2-fold axis at height one forth when applied to this region will fill this space. So, you can see that now, the entire base of the projection is filled, but recall that the height of the all these asymmetric units are only half the unit cell. So, you have actually filled in 3 dimensions in the projection it seems we have filled entire space, but in 3 dimensions we have failed only half the unit cell, because all of these are of half height, look at this instruction here that z is from 0 to half.

So, how do we fill the remaining half above this z is equal to half. So, the region z greater than half can be filled by using we have the symmetry operation and that symmetry operation we can use this mirror here. Now, notice that mirror is actually at height 0, since nothing is mentioned. So, the height is 0. But then we know from our symmetry concepts that any mirror which always repeats at a distance half to the translation perpendicular to it and the translation perpendicular to this mirror image of height C or length C.

So, this mirror which is coming at 0 will also be repeated at half. This information are not explicitly given in the table, but, it is expected that the reader knows these information. So, if we have a mirror at 0 height, we also have a mirror at half height. So, since we have already filled with asymmetric unit, everything up to half height, and then we reflected into this mirror at half height, the upper half will also be filled. So, we have seen that how using different symmetry operations other than translation, we can use an asymmetric unit to fill the entire unit cell.

After this of course, we are free to use translations also, once we have filled a unit cell, we can carry on filling other unit cell simply by translations because translations are also allowed for asymmetric unit. If you do not wish to use translation, it is possible to continue to extend beyond the unit cell even using the rotations and reflections as we were doing. So, thank you very much.