3D Space Groups XI:
Interpretation of International Table Page
Part-4: Origin
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Lecture 25 a

So, we continue our journey in the interpretation of international tables page. So, we go down the page. And in this part, we will discuss the origin.

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So, in part 1, we already looked at the header, which is this part, which gives the basic information about the space group. And then in part 2, we discuss the symmetry diagram, which was this one. In part 3, we looked at the general position diagram, which was this diagram. So, if we continue the journey down the page, the next item, you can is the origin statement, and it is telling origin at the center 2 by m at cc 2 by m. So, let us see, how to interpret this information.
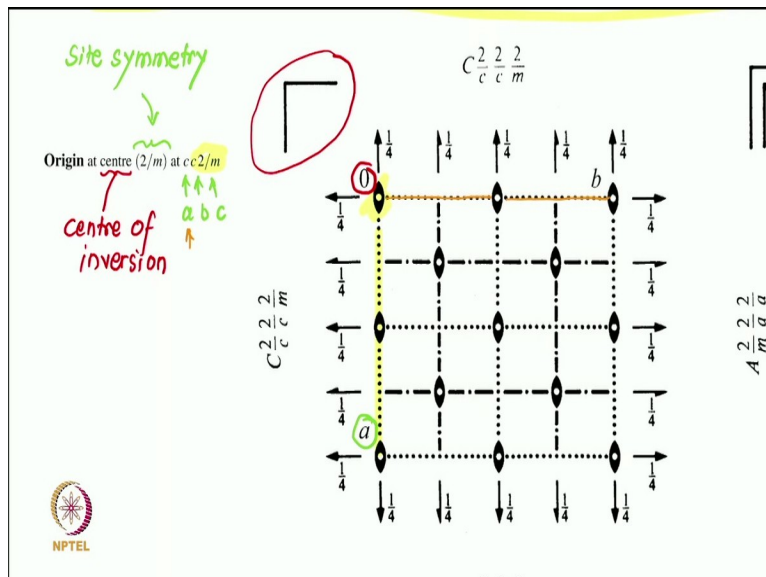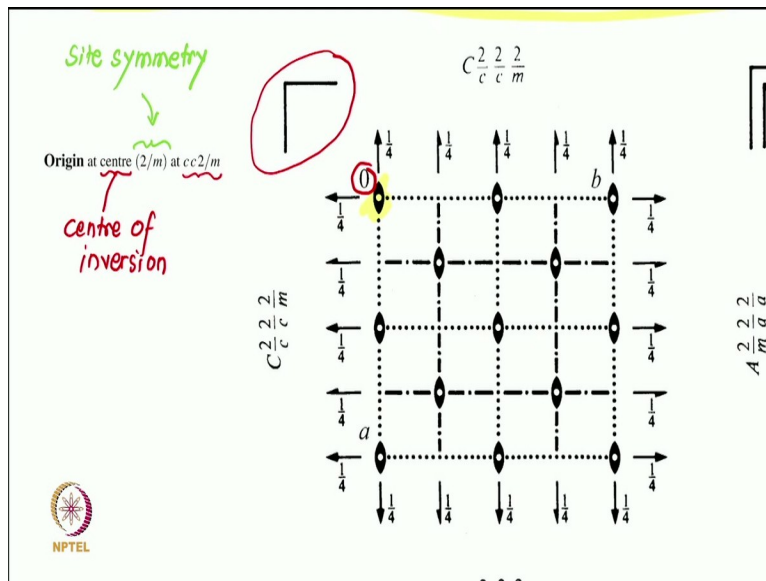
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So, origin statement is very, very important, because for example, the next items as you can see coming is the symmetry operations, so, these symmetry operations data and on the next page, we will see Wycoff projections. So, the Wycoff producing data, these depend upon our choice of origin. So, origin choice is very, very important and has to be paid attention. So, let me just copy this original statement and paste it here for quick reference. So, here I paste it origin at center, this description, and we will try to relate it to the diagram, the symmetry diagram shown here.

So, you can see that by convention, the origin is always taken this O is the origin let me use a different color, O is the origin. So, upper left corner is usually taken to be the origin in the diagram. So, there we have the origin however, one could have chosen origin at other locations. So, the location of the origin is important what is being given here that origin is at

the center, center means center of inversion. You can see that in the symmetry here we have a 2-fold axis shown and inside the 2-fold axis, there is a hole it is not completely black, there is a white dot. So, that white dot represents the center of inversion.

There is more detail about the origin and which is given here. So, it says it gives the site symmetry of the origin. So, site symmetry, it is saying that origin is at 2 by m. So, it is the center but that center is actually at 2 by m, 2 by m means a 2-fold that black lens represents a 2-fold perpendicular to the plane of the projection and by m is a perpendicular mirror, which in this diagram, as you can see, is shown by the symbol here. Because, if the 2-fold is perpendicular to the plane of the mirror, then the mirror itself will be parallel to the plane and in this case, it is passing through the plane it is coinciding with the plane because no height is shown.

So, no height is shown means it is at zero height. That means, it is coinciding with the plane of projection. So, that is a 2-fold axis with a perpendicular mirror plane. Now, there is a further information given here that the cemetery at this location, is c c 2 by m. So, let us see this, this is an orthorhombic group. So, the 3 numbers, the 3 symbols represent correspond to the a axis, b axis and c axis. So, what it is saying that at the origin perpendicular to the a axis, there is a C glide plane. Now, as you can see, this is my a axis.

So, perpendicular to a axis is this plane, and you can see that this plane is shown by dotted lines. So, there is a C glide there. So, perpendicular to the a axis you have a C glide similarly, perpendicular to the B axis also you have a C glide and parallel to the c axis you have 2-fold and perpendicular to the c axis you have mirror plane. So, that is the last item shown there. So, a complete symmetry description and the location of the origin is given in the International Table and one has to carefully study that to make sure that one is aware about the origin of the space group one is working with. Thank you very much.