3D Space Groups X:
Interpretation of International Table Page
Part-3: General Position Diagram

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Lecture 24 c

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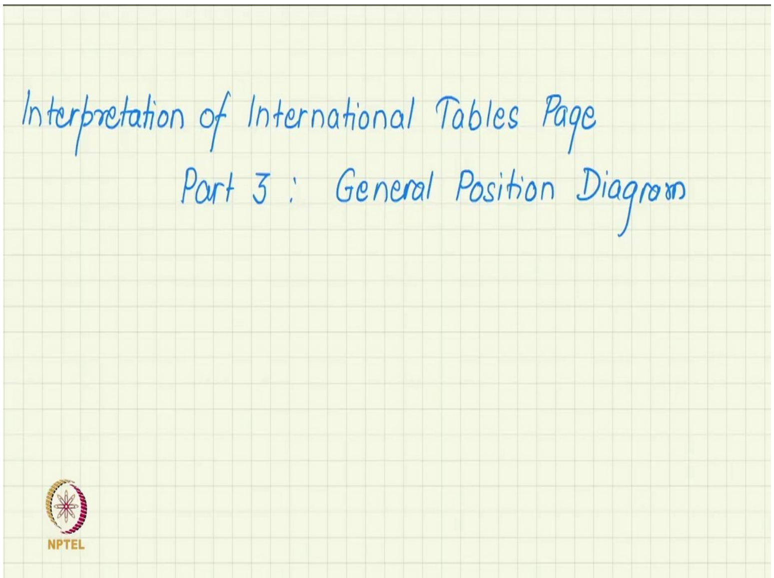

We continue the interpretation of international tables page. So, this is part 3 of the series. And in this video, we will discuss general positions diagram.

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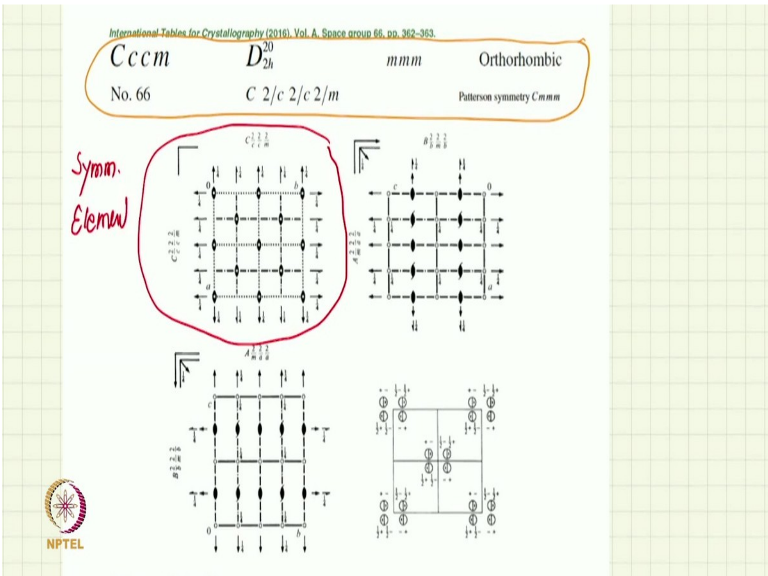

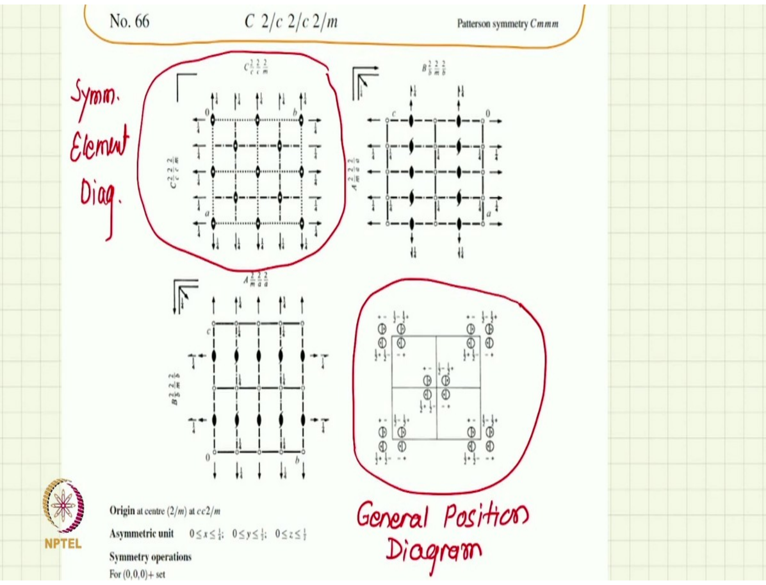

So, this is the space group, which we have been focusing on that is a space group number 66. And in the previous 2 videos of the series, we first discussed the headline. So, the details are given here. And then in the next one, we discussed what is called there are 2 kinds of diagrams given here. One is the diagram which is diagram of symmetry elements, symmetry element diagram and the other one this last one here is general position diagram. Of course, in this space group there are 2 more symmetry element diagrams, which are different projections, as we have seen. So, in the current video, we will focus on the general position diagram.

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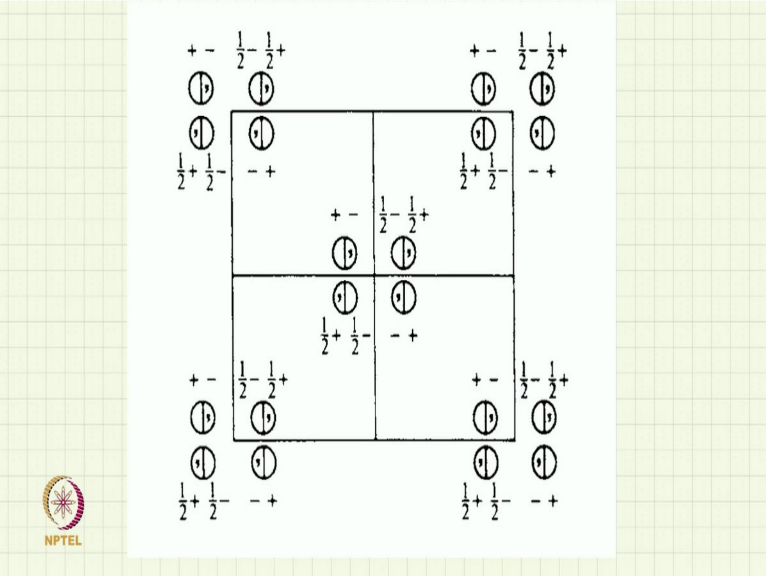

So, this is a magnified view of the general position diagram, you can see where in at one glance, it looks complicated diagram with several circles and commas and plus and minus signs and fractions half plus and half minus. So, what we will do is to build this diagram, now one by one, so as to gain a better understanding.

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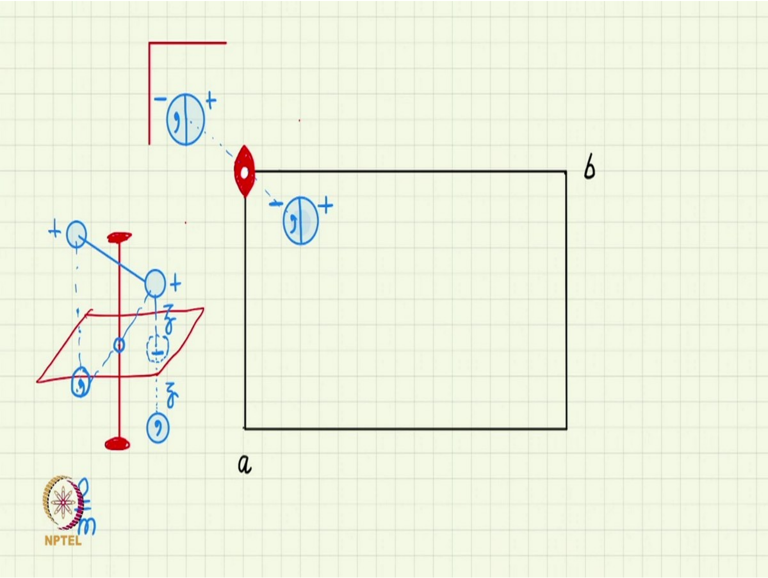

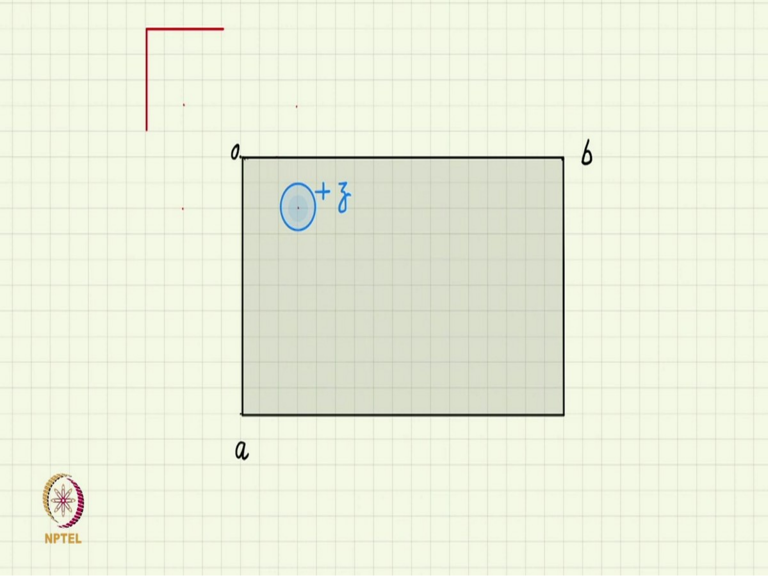

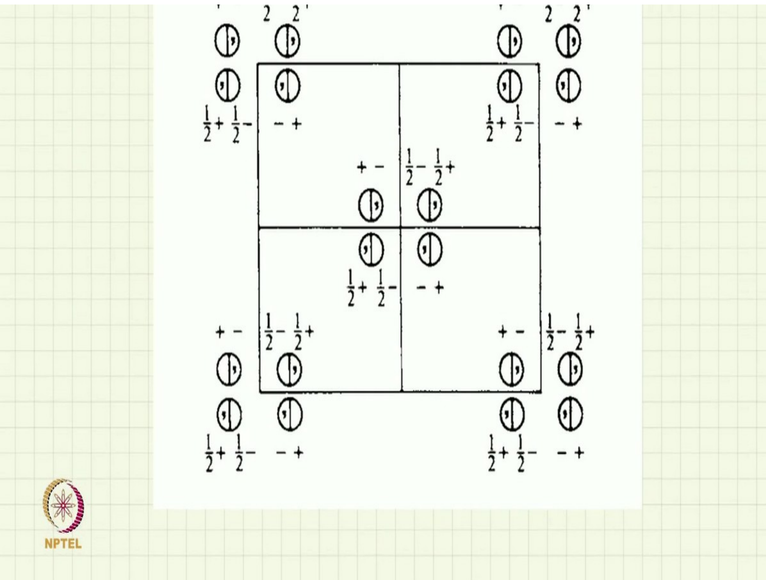

So, I start with an empty unit cell here the projection of an empty unit cell and I have the same projection a-b projection. So, this is the a direction and this is the b direction this is the origin O and we start with what is called a general position. So, what really is meant by a general position that position which is not relying on any symmetry element. So, a general position is a position which does not lie on a mirror plane does not lie on a rotation axis does not lie on an inversion point. And it does not lie on any specific symmetry element.

So, the site symmetry, the symmetry at which the point is located is the identity. So, that is what is called a general position. So that is why I have selected a location like this, because you can see from the symmetry diagram, which we had, you can see the symmetry diagram here. So, I mean to select a position, I am not showing all the symmetry elements there. But you can think of that my circle is somewhere here with respect to the symmetry diagram.

So, that is why it is not lying on any symmetry element. Then, so, that is the starting general position. After that, we have to apply symmetry elements one by one to generate other positions, which are symmetry equivalent. So, recall that one of the symmetry elements of this diagram here, shown here is a mirror plane parallel to or along the projection plane. So, this is shown by these 2 lines at 90 degrees to each other. So, there is a mirror plane and we also give a height c, if this circle if the blue circle is exactly on the projection plane and projection plane is a mirror plane, then obviously this is not a general position.

So, we will have to lift this point up from the projection. So, to lift it up, I give a symbol plus to it, I give a symbol I give a simple plus to it. Plus, here stands for actually, plus z means it is z coordinate it some arbitrary value of z, but it is about the x y plane. It is about the ab plane, and its height about the ab plane is z. But to keep the diagram simple in a z is not required, and only plus sine is given, which means that it has some coordinate about the same height about the x y plane.

Then now let me apply this mirror symmetry to it, as soon as they apply the mirror symmetry, you can see this from a 3D visualization. So, this is my mirror plane, the projection plane. And if this is my general position here, and its height above the mirror plane is z. So, I am writing it as plus, but then if I reflected it will go below the mirror plane. And we will also change the handedness and change handedness in the crystallographic notation is shown by a comma. So, I represented by a comma and below this plane, now, if it was about a height z about the mirror plane, then it will exactly again be a height z below the mirror plane, the image point.

If I project these 2, they will project in the same location. So, in the projection, one has to represent 2 points one above at plus and another below at minus z and the 2 are of different handedness. So, the standard notation used for this is to divide the circle into half, divide the location into half and then show the change in handedness by comma in half of the circle.

So, these 2 circles are representing now, these 2 points as shown in the 3D perspective on the right and instead of plus z now, this is at minus z, which I simply denote by minus. So, I get 2 positions, 2 equivalent positions related by mirror at this location. Let us look at consult the symmetry diagram, another important symmetry is this 2-fold axis with the center of inversion, this 2-fold axis is perpendicular to the mirror plane. And so, in my perspective diagram, that will be a 2-fold axis perpendicular to the mirror plane. And in the projection notation, it is shown like this. And a center of inversion is also if you see the symmetry diagram a center of inversion is also shown by a hole in this lens.

So, I create a hole of course, you know, that this particular side symmetry will be considered as 2 by m. Because there is a 2-fold axis and there is a perpendicular mirror plane and you know that whenever you have a symmetry like 2 by m, the intersection point develop as the center of inversion. So, that is what is being represented there. So, now, what will happen, if these 2 equivalent points which are there, if I apply this 2-fold axis at the origin 2-fold rotation about an axis passing through the origin, if I do that, then I will develop both of these points will rotate by 180 degree.

So, in the projection plane they will go like that. So, you can see here in the 3D drawing if I draw so, it is rotated by 180 degree to that location and then its projection also will its mirror reflection will go that way. So, again in this new location, you will have both the handedness object and the height does not change due to the 2-fold rotation perpendicular to the mirror. So, plus will remain plus, minus will remain minus and left handed will remain left handed and right handed will remain right handed.

So, we will get another 2 equivalent positions there. The the center of inversion is automatically satisfied because you can see the plus here will be inverted to minus below. So, plus above will be inverted by the inversion center to the minus sign, and we will change handedness due to inversion. Now, so, I have 4 equivalent positions now, which satisfy the mirror and the 2-fold, but you can see there are many other equivalent positions here. So, how are they getting generated?

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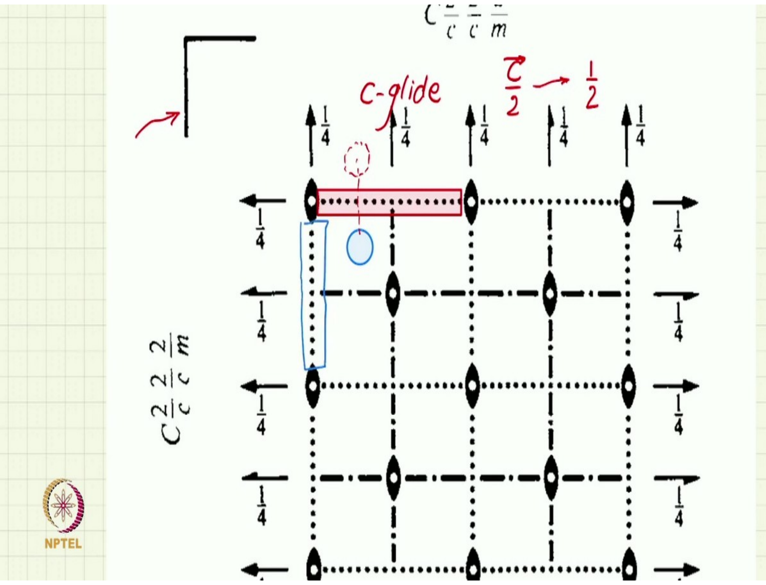
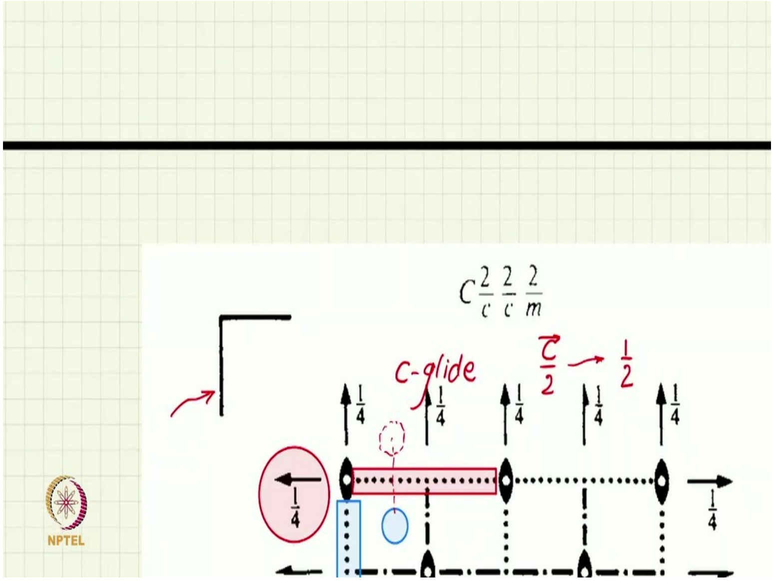
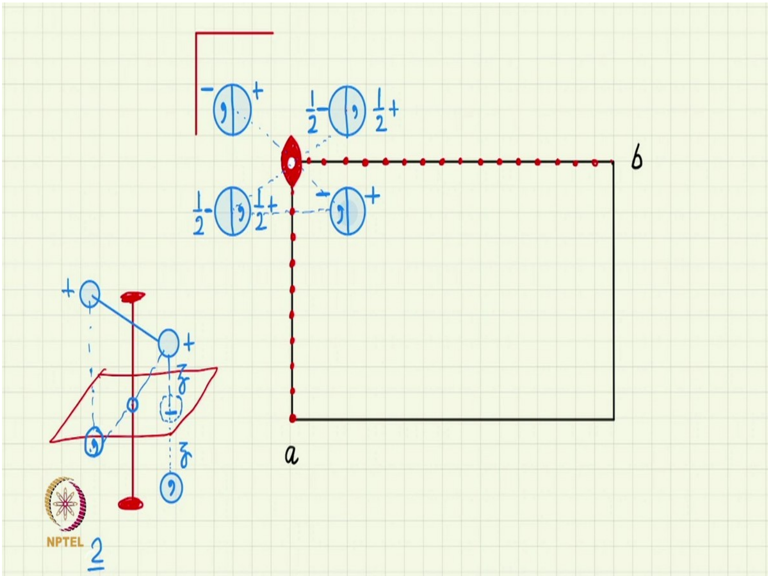



$C\frac{2}{c}\frac{2}{c}\frac{2}{m}$
c-glide
$\frac{\vec{c}}{2} \rightarrow \frac{1}{2}$
$\frac{1}{4}$
NPTEL


a
b
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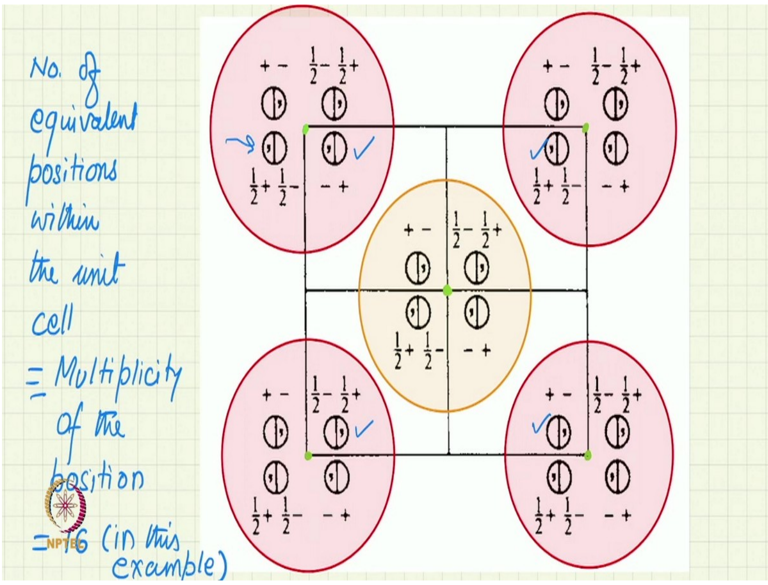
No. of equivalent positions within the unit cell
= Multiplicity of the position
= 16 (in this example)
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So, let us look at consult the symmetry diagram. In the symmetry diagram, we find that one of the symmetry which we have not yet considered is this glide operation. This dotted line is representing a glide operation. And the glide vector since it is dotted, the glide vector is into the plane of the paper or out of the plane of the paper, it is perpendicular to the plane of the paper. So, it is a C glide. And the C glide, the glide vector will be C by 2, which in crystallographic notation in fractional coordinate notation, we will simply represent by half.

So, which means there is a mirror plane there, I will reflect the object into the mirror plane and then translate by C by 2 perpendicular to the plane. So, it will go there and will translate up by half. So, let us do it in the diagram here. So, this plane for first let me try to make this give this the symbol of glide, C glide, C glide by these dotted lines. So, I reflected, reflection takes it there, reflection will change the handedness. So, the right-handed will become left-handed and left-handed will become a right-handed and you can see that if something is z and I translate it further C by 2.

So, it will go from z to z plus half or we can write it as half plus z just like for plus z, we use the shortcut of writing only plus. So, similarly, for half plus z, we will use the shortcut of writing just half plus. Similarly, the minus one will also reflect on reflection the height does not change, it remains at minus z, but then when we translate by C by 2 that is half, so, it would become half minus z which will be represented simply by writing half minus. So, I now have 6 symmetry equivalent adjacent.

All symmetry operations act on all points. So, now, the 2-fold axis which I am showing at the center will act on this newly generated set of equivalent position. So, it will simply rotate it by 180 degree to reach there. So, I can then add 2 more points at 180 degree away without change of handedness and without change of height. So, half plus will remain half plus, half minus will remain half minus. Let me lower this diagram, so, it is not too dotted there. But there are still more symmetry elements have we satisfied all of them? So, you can see that there is a glide here also.

So, what will happen if I apply that glide? You can see that we have already applied that glide because these 2 positions are related by glide, you can see plus which was without comma on reflection will go to half plus and will change the handedness. So, we will have the comma. So, this other glide is an automatic result of the operations which we have already followed, but since it is present in the crystal it is shown there.

Similarly, you can convince yourself that there is one forth 2-fold is already used in creation of these 8 positions. So, in the end these 8 positions satisfy all the symmetry elements in and around that lattice point. So, we have created now, this motif, but there are many other equivalent positions shown in this diagram in the symmetry diagram, those will get generated now, simply by translations because remember that this is a C centered lattice. So, first of all lattice points are at each corner of the unit cell. So, identical motifs will be placed at each lattice point and since it is C centered lattice, so, the center of the base is also a lattice point.

So, again an identical motif is placed at that center of the base. So, then this completes the entire general position diagram, if you count the number of general positions within the unit cell. So, you can see that there are 16 general positions within the unit cell. So, I will be counting I will be counting 2 here 2, 4, 6 and 8 and there will be 8 in the center. So, there are 16 I am not counting for example these because these are outside the unit cell. So, within the unit cell there are 16 positions, the number of positions within the unit cell number of equivalent within the unit cell is called multiplicity of the position. So, this is the general case in this special case, we see that the multiplicity is 16. So, that completes the discussion of general position diagram. Thank you very much.