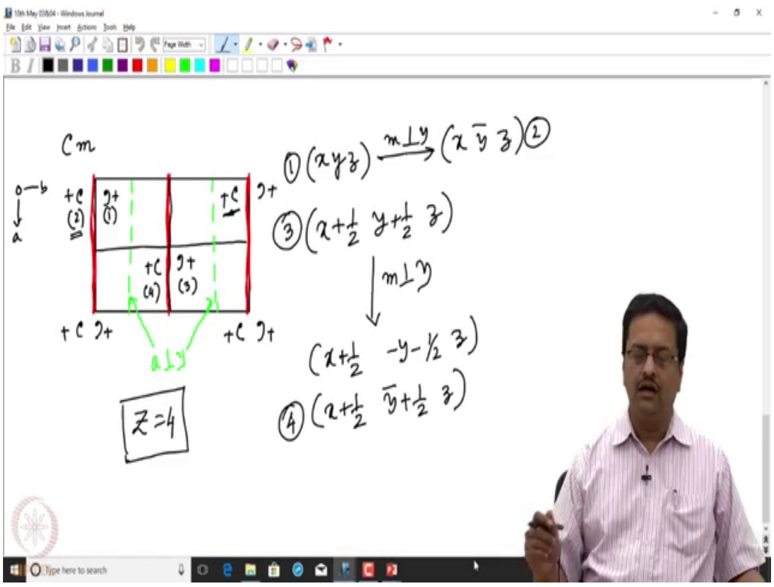
Chemical Crystallography
Prof. Angshuman Roy Choudhury
Department of Chemical Sciences
Indian Institute of Science Education and Research, Mohali

Understanding of Space Groups and Miller Indices
Lecture – 12
3D Space Groups and Equivalent Points

Welcome back to the course of Chemical Crystallography. This is the third week, we are going to start and in this week, I will still continue the discussion on 200 and 30 space groups and how to draw their projections on it, two dimensional plane and using, two dimensional, presentations using pen and paper as I indicated the 230 space groups are subdivided into different crystal systems. And in terms of centric and non centric, there are two types and the non central space groups are further subdivided into chiral and achiral space groups.

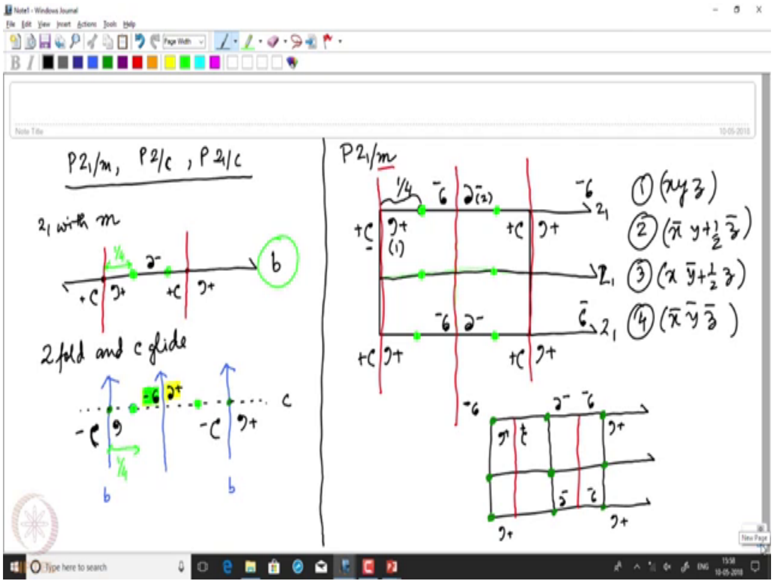
(Refer Slide Time: 01:01)



In the previous lecture, we have seen how to draw the projections for a series of monoclinic, space groups and some of those were centrosymmetric, some were non centrosymmetric and in all the cases, we consider the origin to be at this end corners of the unit cell and the symmetry elements were coinciding with the corresponding origin.

In this lecture, we will see for a particular type of symmetry combinations. The origin cannot be placed in the point of intersection of the two symmetry elements. Such a point which a space groups would include the symmetries like P 2 1 by m, P 2 by c, P 2 1 by c.

(Refer Slide Time: 01:50)



These kind of space groups which are having a combination of twofold with mirror, two fold with glide plane and 2 1 with a glide plane simultaneously. We will see that these combinations of symmetry elements require a shift of origin. Just let us try to see if we combine 2 1 with a mirror, what happens? Suppose, we write the 2 1 screw in this direction and this is my unit edge length units cell, edge length where I have two dots.

So, now, if I have one object somewhere here with plus sign and if I want to do a 2 1 operation on this object which is along the b axis suppose, then what should happen is I will do it to 1 which 2fold should bring the object here with a minus sign; but then since it is a glide, it moves half way along the direction of b and becomes minus as it as it is going below the plane. So, I am erasing this one which is not the real coefficient.

Simultaneously, as I said it is 2 1 with m which is perpendicular to this 2 1 screw, I am trying the mirror at the lattice point which is here. So, because of this mirror, what would happen is that the symmetry related object appears here and the symmetry related object appears there. Now, as we know that 2 by m generates a center of inversion here, it is 2 1 by m and it is generating a center of inversion, but not at the point of intersection of these two symmetries, but it generates the center of inversion in the middle point here. So, that point is at one-fourth unit away from the point of intersection of these two symmetry elements.

Let us see what happens if we have a combination of 2 fold and a c glide. Let us assume that the c glide is from left to right and the unit cell spans from here to an point here. So, if I draw my 2 fold axis, the c glide is perpendicular to b and 2 fold is parallel to b; this is the direction of b. So now, if I take the object, just like before and unit translation takes it there. So, when I am trying to do a 2fold operation, it takes the point below the plane of projection. So, it makes it minus.

The same way symmetry related object also becomes minus here. Now, if I try to apply the c glide which is a reflection followed by translation, so this translation is half translation along the direction c and it remains as plus. The same thing, if we do it for this object which is already mirror related we do a mirror. So, minus becomes inverted minus and then on translation that appears here as minus.

So, what has happened? If we look at it carefully that we have generated a 2 fold symmetry here; so that the points which are this and that are related by 2 fold and simultaneously, we see that the point which is here and the point now which is there are related by the centre of inversion located at this place and once again it is here. You see that the position of this origin is shifted by one fourth with respect to the centre with respect to this 2fold axis this distance is one fourth.

So, this shift of origin has to be brought into to see that the unit cell does not have the center of inversion coinciding with the point of intersection of the two folder, 2 1 screw axis along with the mirror or the glide plane. So, to see that to show that on the right hand side, I am now going to draw the projection of P 2 1 by m. So, for that what I need is a rectangle which represents the AV plane and then I will apply the symmetry elements on this where we have the two 1s. We have the 2 1 screw here and there and now, I am placing my object here which is comma plus and I am trying the translation related objects as usual.

So, now if I do 2 1 operation with these points for my easy understanding, I am dividing this unit cell into four parts. So, that I should place the 2 1 related object at a right place. So, now if I start with point number one and do it 2 1 operation; it comes here with a minus sign. If I do the same for the symmetry related upper point here, it appears at this point.

Now, as I indicated this has a symmetry mirror perpendicular to this 2 1, the mirror is here and the mirror is there as well. So, by doing this mirror operation, what we get here is this for that point. We get one object here, we get one object there, we get one object here. So now, if I once again apply 2 1 on this point, what should happen is it should go up and come somewhere, there with a minus sign same happens to this comes here with a minus sign. This point goes far away with a minus sign and so on.

So, now what do we see is that it has generated a mirror plane in the middle of the in itself and it has generated another 2 1 screw to the midpoint of the medium middle portion of the unit cell through the center of the image. So now, one careful observation what we see that the 0.1, here is my 0.2 centre of inversion appears here, the center of inversion appears, there it appears here and it appears here as well.

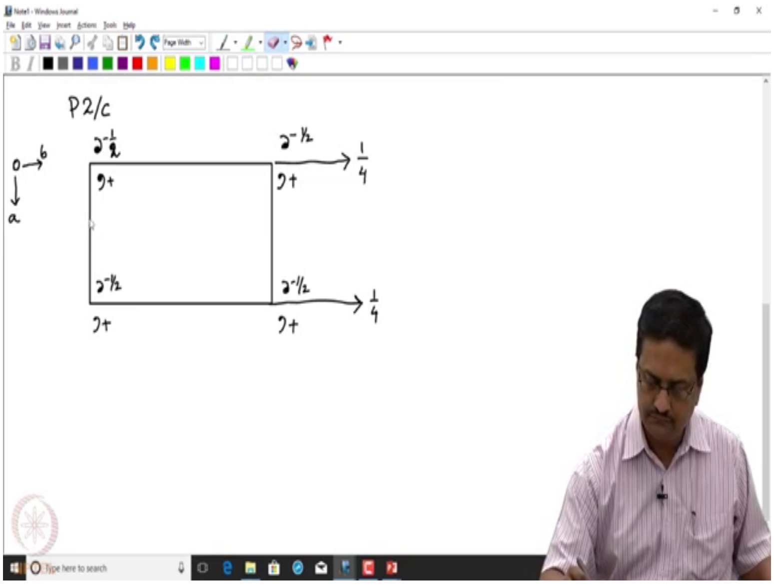
So, now if we understand now that the inversion center is on the 2 1 screw, but it is not coinciding with the mirror which we have seen in the case when we combine 2 1 with a mirror. So, what we need to do is if we shift the origin or if we shift the position of the mirrors, we can re draw this figure in the following manner. These are the translation related objects and the 2 1 as usual is like this and the middle 2 1 is also there.

And now, I am placing the mirror which is one fourth shifted from origin; you can see here, it is one fourth shifted from origin. So, I am placing the mirror which is shifted not on the line here, but it is shifted by one fourth this side and it is shifted one fourth on the other side. So now, if we start putting these symmetry related objects, it should appear like that the 2 1 screw should take the object here with a minus sign and the corresponding mirror image should appear there, the object which is here comes at that point with a minus sign, the corresponding mirror image appears there.

So, the translation symmetry related object of that minus sign appears here; so that means, now the origin is at the corners that are at the eight corners, the center of the faces and here, there and also at the middle of the unit cell as well. This should have been plus, because this is a mirrored operation; so this is plus. So, as we see that this plus gets inverted to minus that class gets invited to minus through the inversion center in the middle of the unit cell.

So, by doing this what are the equivalent points that we have got? Point number 1 is xyz, point number 2 is x bar y plus half z bar, point number 3 x y 2 y bar plus half z and the fourth one is x bar y bar z bar. So, the relationship between 1 and 4 is inversion 2 and 3 is also inversion. I hope you could follow this crystallographic projection of P 2 1 by m.

(Refer Slide Time: 17:35)

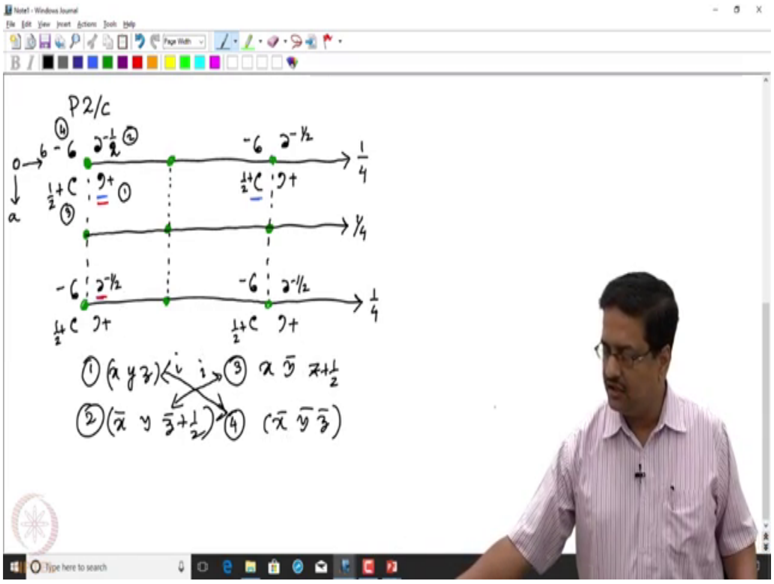


In the same manner, let us now try to do P 2 by c. So, here I have a combination of 2fold and a c glide by 2fold goes here, but these 2fold is not in the plane of projection, but it is one-fourth shifted along c. I hope you remember that we are drawing one b from left to right and o a from top to bottom and c axis is perpendicular to the plane of this board. So, this 2 1 by 2 fold that we are drawing is one-fourth lifted up.

So now, if we have our object of concern here, the symmetry translation, symmetry related objects are placed in the next unit cell as usual that is like in the previous cases,now we are trying to do the 2 1 sorry, 2 fold operation on these points. So, if you apply 2 fold operation on these points; first of all it should go with minus. Since, the 2 fold is one-fourth above the plane of projection; it goes halfway down the plane of projection by doing a 2 fold operation. So, I write it as always minus half.

Now as we see here, there is a c glide. So, if we want to place a c glide then, what would happen is that we should draw c glide like this instead of a bold line and c glide means reflection followed by translation along c.

(Refer Slide Time: 20:16)



So, a point which is on the right hand side of the glide plane comes on the left hand side with a translational component of half in the upper direction. The same thing happens with this point, but it is a half translation it is already half translated and another half translation makes it minus. So, the same point which is here is translated to the other side and the point which is here is translated, here to as a minus sign.

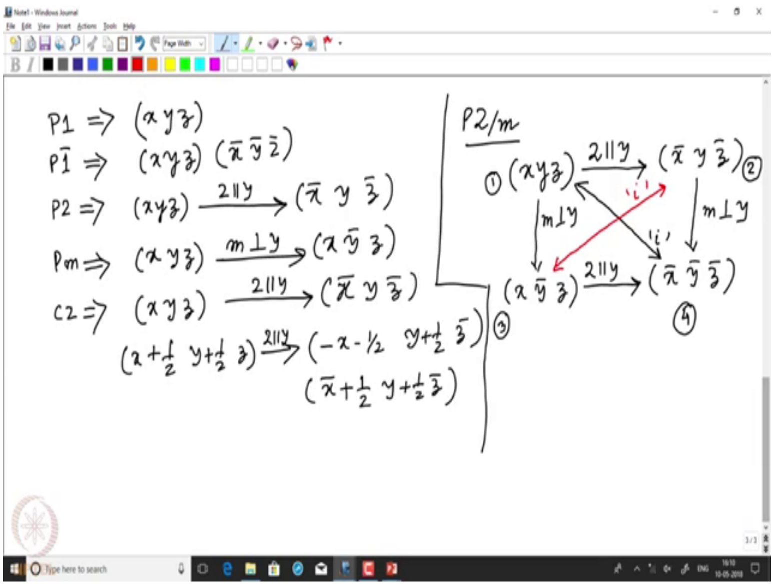
So, as a result what we have got is a center of inversion at a point which is here, there, there and here. So, let us write down the other points which we have not written earlier. In addition to those four inversion centers, see the relationship between this comma plus and comma minus is inversion about the center of the face here, center of the face there, center of the face here, center of the face there and at the center of the unit cell.

Now, you see what is the relationship between the point here and point there? These two points are again related by c glide and that glide lies through the middle of the unit cell which is here. What is the relationship between the points this one and that one? These two points are once again related by a 2 fold passing through the center of the unit cell, but lifted by one-fourth.

So, in this case what we see is that the 2folds are not on the plane of projection rather they are one forth up the mirror plane which goes it is perpendicular to the plane of projection. This mirror is the c glide and hence, the point where the c glide meets the 2, 2 fold axis is not the center of inversion rather the center of inversion is one fourth down compared to the point of intersection. This is what we observe in cases of these specific space groups.

So, what are the equivalent points in this case? I am designating the points with numbers 1 2 3 and 4. So, the equivalent points are xyz x bar y z bar plus half, x y bar z plus half and forth is x bar y bar z bar. So, you see again this points one and four are inversion related, points three and two are inversion related. So, this is how we can draw the stereographic projections of some simple space groups.

(Refer Slide Time: 25:09)



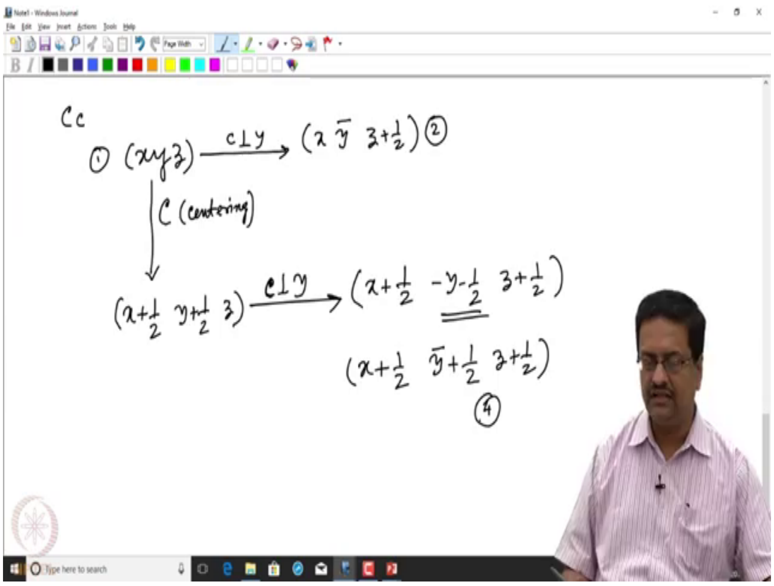
Now, we will see how can we generate the corresponding equivalent points applying symmetry operations only and without drawing the equivalent points. So, in this case we will again start with the simple one P 1 which means there is no symmetry. So, it has only one equivalent point xyz, as we have already learnt. When we go to P 1 bar, we have inversion center in it. So, inversion center means all the coordinates that we have are going to be inverted. So, xyz should become x bar y bar z bar and we have two equivalent points. When we say P 2 this means that we have xyz, then we apply a 2fold parallel to y as a result we end up getting x bar y z bar.

In case of P m we have x y z, we apply mirror perpendicular to y, we end up getting x y bar z and in case of c 2, we have one point xyz; the other point is x plus half y plus half and z. These are the two lattice points in c centered lattice. And when we applied 2fold parallel to y in the first case, we get x bar y z bar; in the second case by applying 2 fold parallel to y, we get minus x minus half y plus half z bar and as I have indicated that minus x, we write as x bar and then when we have minus half, it means the molecule is outside the unit cell, unit cell; to bring it in, we simply add 1. So, when we add 1 to minus half we get plus half y plus half z bar.

Now, let us see if we do it for a simple centrosymmetric lattice like P 2 by m. So, if we start with xyz, we first apply 2 fold parallel to y, we get x bar y z bar. If we apply mirror perpendicular to y on the first point, we get x y bar z and if I now apply 2 fold parallel to y on the third point, we end up getting x bar y bar z bar.

You see here, if I apply mirror perpendicular to y on point number 2, we end up getting the point number 4 which is inversely related to point number 1 and point number 3 is inversely related to point number 2. So, in this case with without any difficulty, we could derive the four equivalent points for P 2 by m space rule. Let us try to derive it for a c centered lattice, which is C c.

(Refer Slide Time: 29:18)



So now in case of C c; we start with point number one which is x y z, we apply a c glide perpendicular to y, when we have c glide it is x y bar z plus half, this becomes point number two; the third point is a c related point compared to the first point it is c centering. So, we should get x plus half y plus half z and then on this we will apply c perpendicular to y, that is c glide perpendicular to y; this is c centering.

So, what we end up is x plus half minus y minus half z plus half, because the translational component is along z. So now, we replace this middle coordinate, that is the coordinate of y like this; y minus y becomes y bar and minus half is removed by adding 1 to this coordinate. So, it becomes plus half z plus half. So, this is the fourth point in the lattice in the space group Cc.

So, in this lecture, in last about half an hour, we have learnt how to draw the space group diagrams for some of the monoclinic space groups with central symmetry non centrosymmetric and we have shown how one can shift the origin when there is a combination of 2 1 bit mirror 2 fold with c glide and 2 1 with c glide and then we started learning how to derive the equivalent points without drawing the space group diagram. We will continue the same in the next lecture as well.