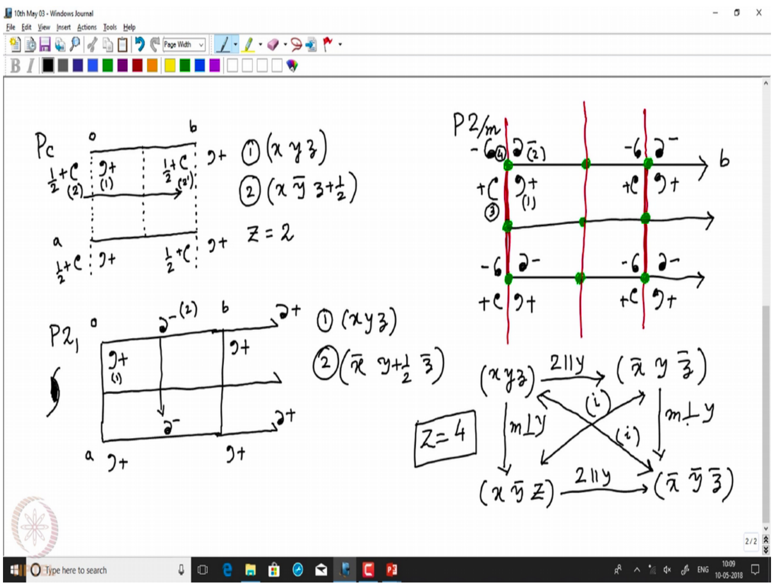
Chemical Crystallography

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

Crystallographic Point Groups and Space Groups
Lecture - 10
2D Projection of Space Groups

Welcome back to this course of Chemical Crystallography. In the previous lecture we have learnt about the 230 space groups and how to understand what kind of space group information is there whether it is belonging to triclinic or orthorhombic or tetragonal or hexagonal and how to identify the lattice centering how to identify the Chiral and Achiral space groups and after that we started understanding how to draw these space groups in a 2 dimensional representation and we have learnt how to do it for P1 P1 bar P2 and P m. So, now let us try to understand the space group pc.

(Refer Slide Time: 01:04)



When we are saying pc it means it is a primitive lattice with a c glide perpendicular to b. So, when I am trying to draw a rectangular lattice I have to keep it in mind that I have a c glide perpendicular to b. So, if the direction from left to right is b and top to bottom is a, the line joining o a represents the c glide which I am drawing as dotted lines. So, this is how one should start drawing these space group diagrams with the understanding of the symmetry that is present.

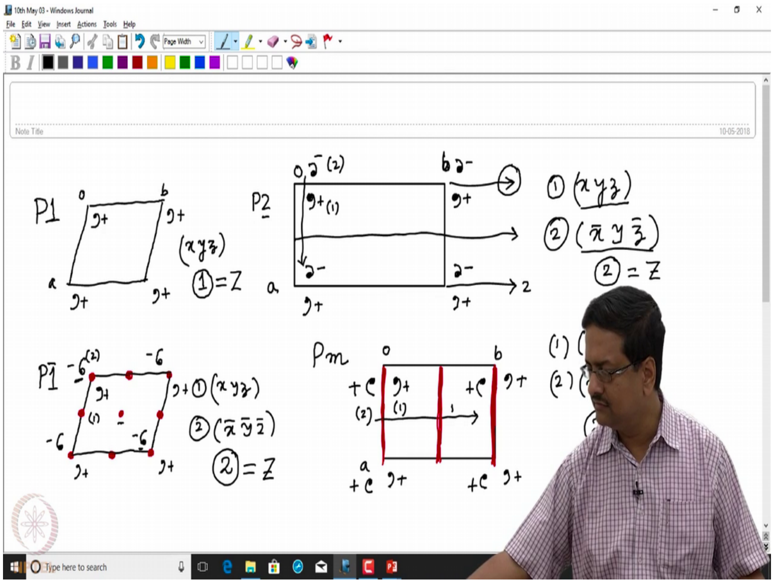
So, now I am drawing the object which may be a molecule or an atom or the group of atoms and the corresponding symmetry related; that means, the translational symmetry related objects I have drawn. So, now when we are saying it is a c glide which means it is a reflection followed by translation. So, the reflection is about the dotted line and the translation is in the direction of c which is above the plane of this particular plane of projection. So, if it was just a mirror we would have written it as this.

But since now it is translated along the c which is the perpendicular direction of this plane of projection and it moves by half unit we should write half along with this object. So, it indicates that it is not only reflected, but also translated half way along the c direction and then we should do the same for all the translation related objects. So, now in this process what has happened the point 1 and point 2 are c glide related objects, if I add 1 along z sorry 1 along b we get the point inside the unit cell. So, now the relationship between 1 and b point which is 2 prime in the inside the unit cell is c glide passing through the middle of the unit cell.

So, what are the equivalent points in this case, the first point is obviously x y z and the second point number 2 is a c glide perpendicular to b; that means, x perpendicular to big brings it y bar and translation along z makes it z plus half. So, what is the value of z here once again it is 2, we have 2 molecules are 2 groups of atoms or molecules inside the unit cell in case of Pc. Let us see 1 mode in monoclinic non centrosymmetric system see in all these cases we have not encountered x y z and x bar y bar z bar so; that means, all these are non centrosymmetric monoclinic space groups.

Now, when I am saying it is P2 1, what I have is a 2 1 screw along b. As I indicated this 2 1 screw when we represent to one screw perpendicular to the plane of projection we represent it with this symbol, but here the 2 1 screw that we are going to represent is along the plane of projection. So, when it is along the direction o b we should represent it as a half arrow, if you had remember the previous slide where we represented a 2 fold with a full headed arrow. Now in this slide we are making it 2 1 as a broken arrow.

(Refer Slide Time: 05:51)



So, now if we try to represent my atom or the group of atom the object, first I am drawing the translation related objects and then trying to apply 2 1 screw. So, now again just like twofold when we apply 2 1 screw the object goes from above the plane to below the plane and here not only rotation of the object there is a translation of the object along b. So, this rotation followed by translation brings the object here with a minus sign, this object which is outside the unit cell down is rotated and translated and it comes inside the unit cell with a minus sign and for the other ones you can have the at molecules translating there.

So, what we have now got is another 2 1 passing through the middle of the unit cell. So, in this case once again this is my at point 1 and that is my point 2 this second point can be translated inside the lattice by adding 1 along a. So, I have 1 as usual x y z and 2 x bar y plus half because, it is translation along y z bar because if it was just a 2 fold axis it would have been x bar y z bar. But it being a 2 1 screw we add a component of half along the direction of translation that is your y.

Now, we would like to see a centrosymmetric unit cell, centrosymmetric space group which is P2 by m; in case of P2 by m what we have is a twofold along the b or the y axis and a mirror perpendicular to b or y axis. So, my object is here 2 fold goes like this along b and the mirror that we have is perpendicular to b which is this surface this face and that face. So, now first thing that we draw are the translation related objects and then we will slowly draw the objects which are related by the corresponding symmetry elements.

First let us apply the symmetry of 2 on all these 4 points when we are applying the symmetry of 2 as usual, if you have the twofold here and the object is here by doing 180 degree rotation it goes to the lowering itself. That means it goes below the plane of projection so the 2 fold object once again comes up here with a minus sign.

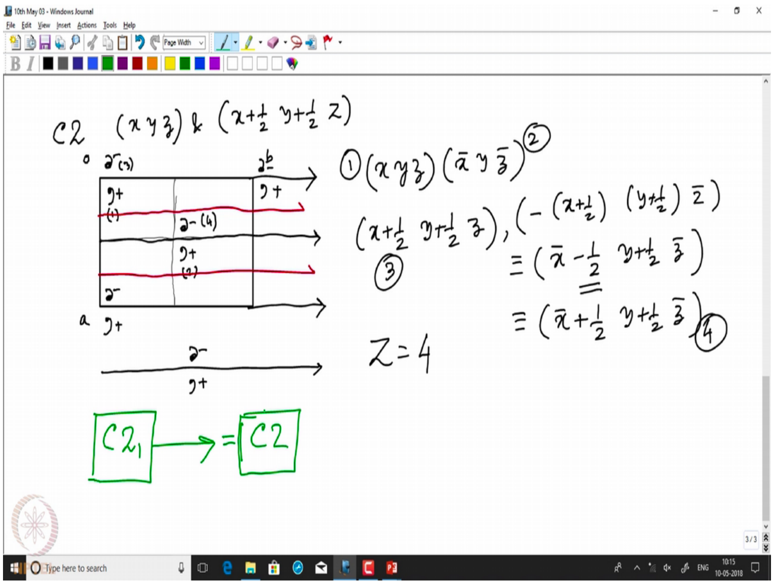
Now, we apply the corresponding mirror if we apply a mirror on 0.1 we get this, if we apply the mirror on 0.2 we get a minus sign on that let me extend the mirror on 2 sides for your better understanding. So, now I am generating the mirror related objects at all the 4 points. Now, what do we see we can see that the point number 1 2 3 and 4 are generated by applying 2 and a perpendicular mirror as a result of that the points 1 and 4 are related by inversion center, similarly 2 and 3 are related by inversion center. So, what we have got our inversion centers at all the 4 corners.

If you look more carefully that the center of the faces are also inversion centers, there is a 2 fold generated through the middle, there is inversion center at the center of the lattice and there is a mirror plane generated through the middle of the unit cell, so this is a complete representation of the P 2 by m space group.

Now let us try to derive the corresponding equivalent points we have x y z, we first apply 2 parallel to y what we get is x bar y z bar, then we apply m perpendicular to y on the point number 1 and we get x y bar z and then either we apply mirror on point number 2 or a 2 fold on point number 3. We end up getting x bar y bar z bar what is the relationship between x y z and x bar y bar z bar is inversion, what is the relationship between x y bar z and x bar y z bar is also inversion.

So; that means this particular space group is centrosymmetric in nature and there are center of inversions located at 8 corners all the 6 faces the center of the faces are inversion centers and also the center of the unit cell is an inversion center. So, you have 4 equivalent points so in this case z is equal to 4. Till now we have talked about only the primitive lattices in monoclinic system, so now we would like to do the same for a couple of centered lattices in case of monoclinic. As you know in case of monoclinic it can be only a c centered lattice. So, we would like to first see what happens when we try to draw c 2.

(Refer Slide Time: 15:28)



As soon as we say c immediately if I have a point at x y z I should also get a point at x plus half y plus half z as it is a c centered lattice. So, now I am going to draw a c lattice here, so in case of a c centered lattice the first thing that I want to do is to divide this unit cell into about a 4 equal parts for my easy understanding; do not get confused because these lines are at the moment do not mean any symmetry element I am just dividing the unit cell into 4 parts, so that I can place the c centered point at correct location.

So, if this is the original point and I start with o b and a as I am drawing here o b is from left to right and o a is from top to bottom. So, when I am going to write the c point which will come here; that means, it is half along a and half along b it comes in the middle of the unit cell, so this is a c lattice. Now the symmetry that we have is a twofold symmetry, so this is the 2 fold symmetry. So, the when we try to draw the translation related objects we should draw them properly.

So, now when we are doing twofold this is minus this is minus this goes as minus and as soon as we have 1 atom at the center we should also have a 2 fold passing through the center. So, this becomes the mirror image sorry the twofold rotated object and this is the 2 fold rotated object here. So, now if I have write this as point number 1 that has 2 or we can write it as 2 and the other one is 3 and this has 4, we have 4 equivalent points what are those 4 equivalent points we start with x y z we apply a twofold on x y z. So, we get x bar y z bar we start with x plus half y plus half z we apply a twofold along the y axis.

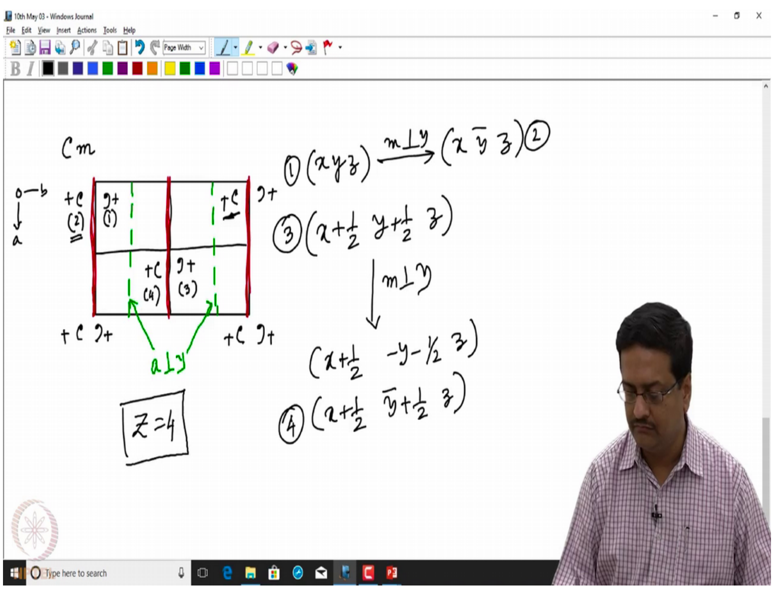
So, the corresponding point should be minus of x plus half y plus half minus z we write it as z bar.

So, now this last point needs to be rewritten as x bar minus half y plus half z bar. So, now you will see that there is a minus half component which indicates that the point is outside the unit cell. So, to bring it inside the unit cell we can add 1 to the x coordinate, so that the atom or the group of atom of the object comes from outside to the in inside unit cell, so we simply add 1 and write it as x bar plus half y plus half and z bar.

So, these are the 4 equivalent points that 1 can derive for the space group C2. What is Z, Z equal to 4 is it centrosymmetric no, the answer is no because, we do not see any inversion center in this what has happened in addition to this C2 the 0.1 and 0.4. If you look at them carefully they also have a different symmetry in between they are related by a 2 1 screw passing through the one forth along a and 3 forth along b. So, this then completes the space group diagram for C2 which indicates that the presence of 2 parallel 2 folds on a c centered lattice gives rise to a 2 1 in between.

I would like you to see yourself what should be the drawing for C2 1, if you try to draw the space group diagram for C2 1 you should yourself find out that it is same as that of C2 and that is why we do not have a different space group called C2 1, but we only represent it as C2. So, now let us see one more c centered lattice in monoclinic system which is c m.

(Refer Slide Time: 22:19)



So, as usual we should first draw the C centered lattice properly, I am trying to divide into 4 equal parts and then placing the object and the C related object, remember always I am representing o b and a in the same direction.

So, now when I am saying it is Cm the symmetry is mirror and that mirror is perpendicular to b, just like pm cm is mirror perpendicular to b. So, if I first draw the translation related objects and then apply the mirror plane. So, this is my point number 1 and the mirror related object is 2, C related object is 3 and the corresponding mirror related object is 4.

So, what has happened here if you look at it very carefully the relationship between 1 and 4 is a reflection perpendicular to b and translation along a. So, reflection perpendicular to b and translation perpendicular along a means it is a glide perpendicular to b. So, as we indicated the symbol for a glide is a dashed line we are drawing that as dashed line, so it is a glide perpendicular to b or perpendicular to y.

So, what are the equivalent points, we started with x y z which is point number 1, we apply a mirror perpendicular to y we end up getting x y bar z that is my point number 2; point number 3 is x plus half y plus half z because, it is a c centered lattice and then on that I am again applying mirror perpendicular to y. So, what we are getting is x plus half minus y minus half z; so that means, it is x plus half y bar and to new this minus half, we add 1 to that because this minus half indicates that this point is outside the unit cell which is here, so I add one along b to bring it at this point.

So, y bar becomes plus half z, so this is the fourth point in the unit cell and as you see that this particular fourth point is not sent inversion related with anybody. So, this is again non centrosymmetric space group with z equal to 4. So, today right now we have discussed about 2 very important space group diagrams C2 and Cm and we have also discussed about P2 by m which is a centrosymmetric unit cell centrosymmetric space group.

So, in the future next class we will talk about slightly more complicated space groups like P2 1 by C or P2 1 by m, where we will see we need to consider the origin shifting from the point 0 0 0 or we need to fix origin at 0 0 0 and translate the symmetry elements; elsewhere otherwise we cannot understand the importance of center of inversion we cannot get the correct representation for inversion related objects.